TOWARDS THE PREDICTION
OF WELD METAL PROPERTIES

by
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VOLUME 1
Mieux vaut prévoir sans certitude que de ne pas prévoir du tout.
It is far better to predict without certainty, than never to predict at all.
J. H. Poincaré, LA SCIENCE ET L'HYPOTHESE.
to

Elizabeth Claire Sugden
PREFACE

THIS DISSERTATION is submitted for the degree of Doctor of Philosophy at the University of Cambridge. The work described was carried out at the Department of Materials Science and Metallurgy, Cambridge, between October 1985 and September 1988.

All the work presented in this dissertation is original work (except where specific reference is made to the contrary), and has not been submitted in whole or in part for a degree or diploma.

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ABSTRACT

A large amount of work has recently been done on the prediction of the microstructure of steel weld deposits, making it possible now to estimate the as-welded microstructure as a function of thermal history and chemical composition. This work is part of a complementary project aimed at obtaining quantitative and widely applicable relationships between weld microstructures and properties.

The thesis begins with a literature review covering the major features of the development of microstructure in low-alloy steel welds, and the recent work on the modelling of this microstructure. A variety of factors influence the relation between microstructure and mechanical properties. The microstructure and properties of a weld are influenced strongly by the mode of solidification, whether this involves the formation of δ-ferrite or austenite as the primary phase, and the solidification stage determines the extent of chemical segregation and growth processes within the weld pool. Experimental work has been carried out to determine the cooling rates at the solid-liquid interface encountered in weld pools as a function of welding conditions. The critical carbon composition for low-alloy steel welds above which solidification will occur as austenite has also been established for the manual-metal-arc process. Thermodynamic models have been employed and developed to allow the various phase transformations experienced by low-alloy steels during equilibrium solidification to be calculated for any reasonable combination of alloying elements. Calculations for the partition coefficients of solute elements during solidification are also presented. This work should provide a basis for the calculation of time-temperature-transformation diagrams for the solidification process.

Detailed models are presented to allow the quantitative prediction of weld metal yield strength, tensile strength, flow stress, strain hardening characteristics, elongation, and reduction of area for a given microstructure and composition. The model for tensile strength is further developed to allow strength to be calculated as a function of temperature. The wide scatter in toughness results often associated with weld metals is shown to be explicable in terms of the inhomogeneity of the microstructure.

Any attempt at modelling the toughness of welds requires a knowledge of the
inclusion distribution. Work on experimental welds has shown that the inclusions in a weld deposit are not uniformly distributed, but segregate to the boundaries of the first phase to solidify. The implications of this work are particularly serious for welds solidifying as austenite, since the inclusions are then located away from the centres of the grains where they cannot act as intragranular nucleants for acicular ferrite. In a separate chapter, fresh evidence that the acicular ferrite phase in welds is bainitic is presented.

In summary, the thesis presents work which has successfully modelled some of the important mechanical properties of welds, and work which has laid the foundations for further research aimed at obtaining quantitative microstructure-property relationships.
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LIST OF PRINCIPAL SYMBOLS

α  allotriomorphic ferrite; alpha ferrite; liquid thermal diffusivity; experimentally determined Charpy constant
α' martensite
αₐ acicular ferrite
αₜ Widmanstätten ferrite
β  constant of proportionality (Barba's law); experimentally determined Charpy constant
γ  austenite; specific interfacial free energy per unit area
γᵢ activity coefficient of solute i (Raoultian standard state and mole fraction basis)
γᵣ retained austenite
δ  delta-ferrite
δₘ solute boundary layer thickness
ε  critical strain; fracture strain
εₑ strain during uniform elongation
ν  number of degrees of freedom
τ  relative plate thickness
Δ₀G^α→γ standard molar Gibbs free energy change accompanying, for example, α → γ transformation in pure iron
Δ₀H standard molar enthalpy change
Δ₀S standard molar entropy change
ΔT temperature deviation from T₀ curve; temperature difference; undercooling
ΔT₀ total undercooling
ΔT₈₅ cooling time through the range 800-500°C
ε  Wagner interaction coefficient
η  coefficient of viscosity
θ  wetting angle; cementite
λ  distance between isotherms
µ  chemical potential
ρᵢ density of an inclusion
ρₖ density of steel; solid density
σ₀ flow stress
GL fraction solidified
$T_o$ curve defining the locus of all temperatures where austenite and ferrite of the same composition have the same free energy.

- $U$: welding voltage
- $V$: volume of particle
- $V_a$: volume fraction of acicular ferrite
- $V_w$: volume fraction of Widmanstätten ferrite
- $V_\alpha$: volume fraction of allotriomorphic ferrite
- $W_s$: Widmanstätten ferrite start temperature
- $X$: mole fraction
- $X_i$: molar solute concentration of component $i$
1.1 INTRODUCTION

Over the last decade, research in welding science has accelerated as a consequence of the increased importance of welding in the fabrication of engineering structures. However, although our knowledge of welding techniques has increased dramatically, the largely empirical approach that has been favoured in welding consumable development has meant that there is still a clear lack of understanding about which factors control the mechanical properties of structural steel weldments for the wide range of welding conditions and consumables which are encountered in practice. Consequently, there is a need for a more theoretical treatment of the subject. The present investigation aims at providing a more formal description of the factors that influence weld metal properties, and is part of a continuing programme whose eventual aim is to quantify the properties of low-alloy steel weld deposits in terms of weld metal chemical composition and thermal history.

As a brief introduction to this field of research, a review of the various aspects of welding metallurgy relevant to this work is now given. Individual topics are developed in the chapters that follow. In this review, following a brief description of arc welding, the essential characteristics of weld metal solidification are discussed, and related to general solidification theory. The current state of knowledge concerning the microstructural constituents that comprise the as-welded microstructure, and their evolution is critically reviewed, and a model that allows the prediction of this microstructure is described. Finally, the significance of reaustenitisation in controlling the microstructure of multirun weld deposits is emphasized. The review highlights many of the key areas in which further research is required, and serves as a good context in which to place the work that follows.

1.2 THE ARC WELDING PROCESS

In arc welding, two pieces of metal are joined together using an electric arc as an energy source, the arc most usually being established between a metal electrode
and the workpiece. The intense heat input causes regions of the joint to melt and fuse together. Manual-metal-arc (MMA) welding with coated stick electrodes is the most widely used of all fusion welding processes, and it is the technique with which this dissertation is primarily concerned. In MMA welding, the arc melts the edges of the component to be welded, and forms a weld pool in the workpiece. Simultaneously, the tip of the electrode melts, and metal drops are transferred via the arc to the workpiece (see Figure 1.1). Melting of the coating on the electrode causes a shielding gas to develop, and this protects the weld from oxygen and nitrogen in the air. The metal droplets which are transferred in the arc are covered with molten slag. On contact with the weldpool, the slag floats to the surface thus providing a protective cover on the top of the hot weld metal.

In the submerged-arc (SA) welding process, which is also widely used, the same principles apply, but the arc and metal are shielded by a blanket of granular fusible material on the workpiece during welding (Figure 1.2).

1.3 WELD METAL SOLIDIFICATION

The evolving microstructure in fusion welding is strongly influenced by the prevailing thermal conditions, and weld metal chemistry. Weld pool conditions are such that growth is nearly always cellular or, in more highly alloyed steels, cellular-dendritic. Under these conditions, the total undercooling is not only a function of the structure of the interface, but is also dependent upon the growth rate and temperature gradient in the liquid ahead of the growing interface. Thus, the total measured undercooling may be written as (Davies and Garland, 1975)

$$\Delta T = \Delta T_D + \Delta T_r + \Delta T_K$$  \hspace{1cm} (1.1)

where $\Delta T_D$ is the contribution due to the solute layer, that is, the undercooling required to give a sufficient composition difference to drive diffusion.

$\Delta T_r$ is the undercooling due to interface curvature,

and $\Delta T_K$ is a kinetic contribution.

$\Delta T_K$, for metals, is usually assumed to be negligible compared to other contri-
Figure 1.1: Schematic diagram of the MMA welding process. (After B. Lundqvist (1977), “Sandvik Welding Handbook”, Sandvik AB, Sandvikken, Sweden, 28).

Since the melt has approximately the same composition as the base metal, wetting of the base metal is very efficient, and the wetting angle, $\theta \approx 0$. This effectively reduces the energy required for nucleation to a point where there is almost no barrier to solidification, and it is only when inoculants are introduced into the weldpool that heterogeneous nucleation theory needs to be taken into account. The base metal acts as a very efficient heat sink, and solidification nuclei form at the oxide-free surface of the melted-back base material. Since heterogeneous nucleation is not expected in weldpools, the chill-cast layer characteristic of ingots cast in moulds is eliminated.

During solidification, certain grains at the base metal will be better oriented than others for $<100>$ growth with respect to the isotherms of the melt, and, in a way exactly analogous to the competitive growth found in ingot solidification, these quickly predominate and widen at the expense of others. The initial low rates of crystal growth are associated with a relatively planar solidification front. As the thermal gradient towards the centre of the pool decreases, the growth rate increases, and the morphology of the front changes through cellular to cellular-dendritic. Even independent nucleation of dendrites ahead of the solidification from may occur. It should be noted that dendritic and cellular substructures in welds tends to be on a finer scale than those in castings. This is mainly due to the comparatively high solidification rates of weld metal.

The cell spacing will affect the degree of solute segregation at the cell or dendritic boundaries with finer spacings giving less segregation. This segregation is a consequence of solute accumulation in grain-boundary grooves. The important factors in determining its magnitude are:

(i) The density and spacing of the cell boundaries,

(ii) the partition coefficient of the solute,

and (iii) the total amount of solute present (Easterling, 1983).

Most rapid weldpool solidification occurs at the centre of the bead, which would thus be expected to have the finest solidification substructure. The actual size of the cellular substructure is found to increase linearly relative to the reciprocal
of the thermal gradient at the solid-liquid interface (Savage, 1980). The general coarseness of the microstructure at the fusion boundary is largely determined by the initial grain size of the base metal. Unfortunately, the base metal at the transition zone receives the most severe thermal cycle, and the grains in this zone tend to grow and become relatively coarse.

The speed of welding has an important influence on the eventual weld microstructure. During welding, growing crystals will try to follow the steepest temperature gradients. The maximum temperature gradient in a weldpool is normal to the pool boundary at all points of the boundary, and the distance between isotherms is inversely proportional to the welding speed. Thus, the form of the competitive growth process in a given material is uniquely controlled by the weldpool geometry.

The effect of increasing the welding speed is to change the shape of the weld from an elliptical shape to a narrower tear shape. A tear-shaped weldpool, (Fig. 1.3a) maintains fairly constant thermal gradients up to the weld centreline because of the more angular geometry of the weld. On this basis, crystals are not required to change their growth directions as at slower speeds, and appropriately oriented crystals stabilise and widen, outgrowing crystals of less favourable orientation. With an elliptical weldpool, as shown in Figure 1.3b, the progressive change in the direction of the maximum thermal gradient is reflected in the survival of many more columnar grains. Since the maximum temperature gradients are constantly changing direction as the heat source moves away, the growing columnar crystals are faced with the necessity of trying to follow the maximum temperature gradients while still maintaining their preferred <100> growth direction. Consequently, a columnar grain which survives over any great distance in a weldpool exhibits considerable curvature due to the progressive change in the favoured growth direction. The crystallographic orientation of the grain is maintained by repeated side-branching of the solidification substructure. If such growth becomes difficult for a number of adjacent grains due to the relative orientation of the easy growth direct and the continually changing direction of the maximum thermal gradient, a new columnar grain may be initiated from a random solid fragment incorporated into the interface from the melt. This fragment will have a <100> direction oriented parallel to the direction of the maximum thermal gradient at the moment of solidification.

Once started, columnar growth normally dominates weldpool solidification.
Figures 1.3a and b: Schematic diagrams showing competitive growth with (a) a teardrop shaped weldpool, and (b) an elliptical weldpool. (After W. F. Savage (1980), *Weld. World*, 18, 93).
However, high welding speeds have been found to be particularly associated with a transition from predominantly columnar crystal growth to equiaxed growth at the final stage of solidification. This transition is thought to be due to the high amounts of segregation associated with the final stages of weldpool solidification. The shallow thermal gradient at this stage leads to high degrees of constitutional supercooling, and therefore the driving force for random dendritic growth to occur is large. This is compounded by the higher welding speeds which tend to cause overlap of the regions of solute accumulation ahead of the converging solidification front at the centre of the characteristically pear-shaped pool.

1.4 THE AS-DEPOSITED MICROSTRUCTURE

During the solidification of steel weld metals, solidification occurs either as δ-ferrite followed by the formation of austenite, or as austenite directly. (This behaviour is discussed in Chapters 2 and 4). In the former case, the austenite grains will usually be on a finer scale than the δ-ferrite columnar grains indicating that, on average, more than one nucleation event occurs at the δ-ferrite grain boundary during the transformation (Widgery and Saunders, 1975). Growth is anisotropic along the grain boundaries and results in a columnar austenite grain structure resembling that of the original δ-ferrite.

The final microstructure of the low-alloy steel weld evolves during the γ → α transformation when a variety of microstructural constituents may form, depending upon the chemical composition and cooling rate. However, the most important are allotriomorphic ferrite, Widmanstätten ferrite, and acicular ferrite. It should be noted that in the past, allotriomorphic ferrite has sometimes been referred to as proeutectoid ferrite or grain boundary ferrite, but these appellations do not differentiate between allotriomorphic ferrite and Widmanstätten ferrite, both of which can form above the eutectoid temperature, and at austenite grain boundaries.†

1.4.1 Allotriomorphic Ferrite

Allotriomorphic ferrite (α) usually forms between 1000 and 650°C during the cool-

† The very many terminologies which have been used to classify weld metal microstructures have been satisfactorily reviewed by the Japanese Welding Society (1983). The subject is not elaborated here, since such classifications are not based on transformation kinetics.
ing of steel weld deposits. Nucleation occurs heterogeneously at the austenite grain boundaries, often with one interface assuming a rational orientation relationship with the austenite. The adoption of a second one with the neighbouring grain resulting in faceted allotriomorphs on the grain boundary. Subsequent growth is extremely rapid, with the allotriomorphic ferrite forming an almost continuous layer of polycrystalline ferrite.

Allotriomorphic ferrite appears to grow in weld deposits without the redistribution of substitutional alloying elements during transformation (whose concentration will be low anyway). The growth rate is thus controlled by the diffusion of carbon into the remaining austenite (Bhadeshia et al., 1985a). This mechanism of growth is termed paraequilibrium (Hillert, 1969), and occurs as a consequence of the fast cooling rates experienced by welds.

Allotriomorphic ferrite is perceived as being detrimental to the toughness of welds. This can be attributed to its relatively coarse grain size, and also its morphology, the continuous layers of which provide minimal resistance to crack propagation (Levine and Hill, 1977; Tweed, 1982).

1.4.2 Widmanstätten Ferrite

Further cooling results in the formation of Widmanstätten ferrite (\(\alpha_w\)). Primary Widmanstätten ferrite nucleates directly from those regions of the austenite grain boundaries not covered by allotriomorphic ferrite. Secondary Widmanstätten ferrite nucleates on the allotriomorphic ferrite grains at the \(\alpha/\gamma\) boundaries. The phase grows as sets of parallel plates separated by thin regions of austenite. Ultimately, the austenite remains in the weld as retained austenite, martensite and degenerate pearlite, known collectively as microphases (see below). The characteristic microstructure of Widmanstätten ferrite and microphases is referred to in welding institute nomenclature as "Ferrite with Aligned-Martenite-Carbide" (Figure 1.4).

Widmanstätten ferrite is the product of a displacive transformation, yet is able to form at low undercoolings below \(Ae_3\) by the cooperative growth of pairs of back-to-back plates whose shape changes largely cancel each other out (Bhadeshia, 1980). The characteristic wedge shape is a consequence of the slight misorientation of the habit planes of these two variants.
carbide in form of bainite, showing dark rugged needles

martensite in form of angular light-grey grains

retained austenite in form of angular grains

Widmanstätten ferrite is perceived to be an undesirable constituent in weld deposits because of its inferior toughness properties (Devletian and Wood, 1983; Taylor and Farrar, 1975).

1.4.3 Acicular Ferrite

Acicular ferrite ($\alpha_a$) is peculiar to steel weld metals, and forms within the columnar austenite grains in competition with Widmanstätten ferrite. Optically, it appears as a fine-grained interlocking array of non-parallel laths, as shown in Figure 1.5.

Until recently, the identity of the acicular ferrite phase had not been established. Recent work (Strangwood and Bhadeshia, 1987; Yang and Bhadeshia, 1987), however, has shown that acicular ferrite is bainite. The acicular ferrite plates form by a diffusionless and displacive transformation immediately after which, carbon is partitioned into the residual austenite. The transformation does not then obey the lever rule, and exhibits an incomplete reaction phenomenon, wherein the reaction ceases well before the residual austenite achieves its equilibrium carbon concentration.† Acicular ferrite differs morphologically from classical sheaf-like bainite firstly because it nucleates intragranularly, either on inclusions, or sympathetically on pre-existing plates, and secondly because growth is limited by physical impingement with other plates which form on neighbouring sites.

Acicular ferrite is a highly desirable constituent in steel weld metals. The large number of non-parallel grain boundaries hinder crack propagation, and impact good toughness to the weld (Widgery, 1974; Garland and Kirkwood, 1975; Taylor and Farrar, 1975). However, as with the other constituents of the microstructure, quantitative information as to its individual contribution to weld metal strength and toughness would be desirable.

1.4.4 Microphases

A fourth category of microstructural constituent are microphases, which are the last constituents to form in the weld. Microphases correspond to the small carbon-rich regions in the weld where the last remaining volumes of austenite transform, and consist of mixtures of martensite, carbides, degenerate pearlite, bainite, and retained austenite. As well as being located between the parallel plates of Widmanstätten ferrite, they form among the non-parallel plates of acicular ferrite.

† This is discussed at length in Chapter 10.
Figure 1.5: Acicular ferrite and allotriomorphic ferrite in a low-alloy steel weld deposit.
From the nature of the transformation products which comprise microphases, it is evident that a high volume fraction will have an adverse effect on weld metal properties.

1.4.5 Idiomorphic Ferrite

Idiomorphic ferrite, which was first defined in the Dubé classification (1948) has a roughly equiaxed morphology and forms intragranularly. It is sometimes believed to form in steel welds when it is often classified as intragranular polygonal ferrite (Duncan, 1986). However, no evidence has been produced that it does not arise as a consequence of sectioning effects, and, in any case, the volume fraction in welds is always small and usually nil.

1.5 INCLUSIONS

Inclusions in weld metals primarily originate from oxides formed during weld deposition, or from the unintentional trapping of slag-forming materials which are used to protect the molten metal during welding. Non-metallic inclusions can be classified into three types. Primary indigenous inclusions are those deoxidation products which form if the saturation point of the inclusion-forming elements is exceeded during cooling, and have dimensions ranging from 1 to $3\mu m$. Secondary indigenous inclusions form as a consequence of the enrichment of the intercellular liquid that occurs during solidification. These particles are effectively trapped in the weld metal. They are characteristically much smaller than primary indigenous inclusions, having dimensions of the order of $0.5\mu m$, although unlike primary indigenous inclusions, their size is strongly dependent upon the cooling rate. The third type are exogenous inclusions. These are comparatively large non-metallic particles of external origin, up to $10\mu m$ in diameter, which are picked up during the welding process, usually from the consumable or the slag, and become entrapped in the steel (Craig et al., 1979). Exogenous inclusions are particularly undesirable, making for low weld metal toughness (Judson and McKeown, 1982). The mean inclusion diameter in low-alloy steel weld deposit can typically be about $0.3\mu m$ (Dolby, 1983; Abson, 1978), although some inclusions as large as $1\mu m$ (Steel, 1972) are sometimes found. The chemical compositions of inclusions are very complicated and depend on the particular welding process used.

It has often been suggested in the literature that a high inclusion volume frac-
tion should lead to a decrease in the austenite grain size of a weld deposit as a consequence of grain boundary pinning. Cochrane and Kirkwood (1979), Barritte et al. (1981), Harrison and Farrar (1981), and Ferrante and Farrar (1981) all reported experiments in which welds with different oxygen concentrations were reheated into the γ phase field and held there to allow coarsening. The resultant equiaxed grains were found to decrease in size with increasing oxygen content, and, since the volume fraction of inclusions in a weld correlates strongly with the total oxygen content, since most of the oxygen is present as oxides, and since most inclusions are oxides, the inference was that inclusions can restrict weld metal grain size. However, their experiments are not relevant to the as-welded microstructure, since they deal with reheating weld metal, when the austenite grain size is controlled by coarsening and driven by the γ/γ surface energy per unit volume, a driving force amounting to only a few J/mol. In contrast, the driving force for the formation of austenite from δ-ferrite is relatively large compared to the force required to pin boundaries, and increases indefinitely with undercooling below the equilibrium transformation temperature. In such circumstances, pinning is not tenable (Yang, 1987).

Inclusions act as stress-concentrators in weld metals, and their rôle in weld metal fracture is well documented (Tweed and Knott, 1983; Knott, 1984; McRobie, 1985). Accordingly, it is desirable that their volume fraction should be kept to a minimum. However, further to this, it is now recognized that the size, type, and even size distribution of the inclusions is important (Cochrane and Kirkwood, 1979; Ferrante and Farrar, 1982; Cochrane, 1983). Although they are a prerequisite for the nucleation of acicular ferrite, above a low critical volume fraction they are unlikely to alter materially the volume fraction of acicular ferrite in a weld (Oldland, 1985). Thus, it is found that the model due to Bhadeshia et al. (1985a) discussed below can predict the volume fraction of acicular ferrite in a weld without a knowledge of the inclusion population.

### 1.6 A MODEL FOR THE AS-DEPOSITED MICROSTRUCTURE

In 1985, a model was proposed by Bhadeshia et al. (1985a; 1985b) by which the microstructure of the fusion zone of a weld metal might be estimated as a function of a few key welding variables. Subsequent work (Svensson et al., 1986, Gretoft et al., 1986, Bhadeshia et al., 1987) has been shown this model to be extremely
successful, and it is now possible to predict quantitatively the volume fractions of the phases present in the as-deposited region of an MMA weld for a given chemical composition and set of welding variables. An outline of the model is given below.

The model assumes the prior austenite grains to have the morphology of space-filling hexagonal prisms, and Figure 1.6 shows one such grain in cross-section. The first stage during the decomposition of austenite is the formation of a uniform layer of allotriomorphic ferrite at the austenite grain boundaries. This is followed by the growth of Widmanstätten ferrite from the austenite boundaries as depicted in the second hexagon. Then, depending upon the growth rate of the Widmanstätten ferrite, it either impinges with the allotriomorphic ferrite on the other side of the grain, or with acicular ferrite nucleated on inclusions (depicted as black dots in Figure 1.6) within the grains.

Figure 1.7 illustrates the steps involved in the calculation of microstructure. With a knowledge of the chemical composition of the weld, and an estimation of the amount of solute segregation in the microstructure, thermodynamic theory allows phase diagrams and TTT curves to be calculated for solute-enriched and solute-depleted regions of the microstructure using a computer program developed by Bhadeshia (1982). The calculations are valid for up to 5wt% total alloying element additions of C, Mn, Ni, Cr, Mo and V, providing all alloying elements stay in solid solution.

From the TTT curve, a CCT curve is derived using an Additive Reaction Rule (Christian, 1975), which allows the martensite, bainite, Widmanstätten ferrite and allotriomorphic ferrite start temperatures, respectively $M_s$, $B_s$, $W_s$ and $T_h$, and the allotriomorphic ferrite finish temperature, $T_f$, to be calculated. Knowing the allotriomorphic ferrite half-thickness, $q$, and the cooling rate of the weld over the temperature range $800 \rightarrow 500^\circ C$, the time taken for the weld to cool from $T_h$ to $T_f$, $t_1$, can be calculated (Svensson et al., 1986), and the volume fraction of allotriomorphic ferrite, $V_\alpha$, is then estimated from the geometry of the grains, ignoring their ends since their length is very much longer than their widths.

Initially it was assumed that the nucleation of allotriomorphic ferrite was not a critical step, so that the formation of allotriomorphic ferrite essentially involves the diffusional thickening of layers of grain boundary allotriomorphic ferrite (Bhadeshia et al., 1985b). However, in some relatively heavily alloyed welds, this is unjustified

Figure 1.8: Diagram illustrating the growth of allotriomorphic ferrite as (a) the normal migration of the $\alpha/\gamma$ interface, and (b) in the case of reality. (After H. K. D. H. Bhadeshia, L.-E. Svensson, and B. Gretoft (1987), "Welding Metallurgy of Structural Steels", [Proc. Conf.], Met. Soc. A. I. M. E., Warrendale, Pa. 15086, 521).
since discontinuous layers of allotriomorphic ferrite are observed (Bhadeshia et al., 1986). This is illustrated schematically in Figure 1.8. The model has since been refined to take account of allotriomorphic ferrite nucleation where site saturation does not occur at an early stage (Bhadeshia et al., 1987).

Currently, the calculated volume fraction of allotriomorphic ferrite is approximately half that actually observed, and the theoretical volume fraction, $V_\alpha$, is modified from the calculated volume fraction, $V_\alpha(\text{calc})$, as

$$V_\alpha = 2.04\{V_\alpha(\text{calc})\} + 0.035 \quad (1.2)$$

However, this calculation for $V_\alpha$ has been found to be very accurate at explaining the volume fraction of allotriomorphic ferrite in the primary microstructure with a correlation of 0.97 on the alloys analysed (Bhadeshia et al., 1985a).

The volume fraction of microphases, $V_m$, can be estimated to a good approximation from the maximum volume fraction of martensite that can be observed from the untransformed austenite at the martensite start temperature, the latter being calculated assuming maximum growth of $\alpha$, $\alpha_w$, and $\alpha_a$.

At $t = t_l$, the formation of Widmanstätten ferrite begins. The volume fraction is estimated by considering nucleation at the $\gamma/\alpha$ interfaces, of which only a certain area fraction can nucleate. The $\alpha_w$ grows sufficiently fast that growth may be treated as an isothermal process, based on a growth rate derived from Trivedi (Trivedi and Pound, 1969; Trivedi 1970a; 1970b).

By calculating whether $\alpha_w$ grows with or without hard impingement with acicular ferrite within the austenite grains, i.e. if the time required for $\alpha_w$ to grow across the austenite grains, $t_3$, is less than a critical time, $t_c$, the volume fraction of acicular ferrite can be estimated by

$$V_\alpha = 1 - V_\alpha - V_w - V_m \quad (1.3)$$

Thus, the volume fraction of allotriomorphic ferrite, Widmanstätten ferrite, acicular ferrite and microphases in a weld can be estimated. Although, this model contains a number of approximations, it is fundamentally sound and predicts the
as-deposited microstructure with reasonable accuracy.

1.7 REAUSTENITISATION

In multirun weld deposits, the weld metal may be subject to not one but a series of thermal cycles of varying severity. Subsequent layers will reaustenitise part or all of those directly below them, with a consequent modification of structure. This additional transformation gives a characteristic microstructure consisting of approximately equiaxed grains, the coarseness of which increases with higher austenitisation temperatures, giving an increasing grain size up to the fusion boundary (Figure 1.9). Welding terminology is not clearly defined, and the reheated region may be referred to as the tertiary microstructure (Hoekstra et al., 1986), or, as in this text, the secondary microstructure, depending upon whether one wishes to regard the as-welded microstructure as primary or derivative.

The secondary microstructure typically has a higher toughness and a lower strength than the as-welded microstructure, and research at Cambridge (Yang, 1987; Reed, 1988) is now particularly concerned with the construction of a model that will allow the prediction of the grain size, and explain the development of microstructure in this region. This is probably a prerequisite for the analytic prediction of the microstructure of multirun weld deposits.

The nucleation of austenite will be dependent upon the chemical composition and initial microstructure of the weld, and the severity of the weld thermal cycle. Its growth will depend upon the diffusion of carbon into the advancing interface. An exciting development has been the design of almost completely reheated high-strength multirun weld deposits, which exploit the good mechanical properties bestowed by reaustenitisation (Svensson and Bhadeshia, 1988). Careful alloy additions are used to produce a weld metal with an \( Ae_3 \) temperature sufficiently low that subsequent passes give a large volume of reheated material, and sufficient hardenability to give a tough, mechanically homogeneous, microstructure. The resultant weld exhibited an unusual combination of high strength and high toughness.

1.8 SUMMARY

This review has outlined the major factors that influence the development of micro-
Figure 1.9: Detail of a multirun weld deposit, illustrating the progressive refinement of weld metal grain size that occurs in the microstructure immediately beneath the weld run.
structure in the fusion zone of low-alloy steel weld deposits. Following transfer of
the molten metal through the plasma of the arc, weld metal solidification is ob-
served to occur at the parent metal interface. Although, the precise morphology
of the solidifying interface is a function of the supercooling in the weldpool, grain
growth is usually in the form of columnar grains, and this leads to an inhomoge-
neous distribution of alloying elements within the weld. At lower temperatures,
decomposition of austenite in the weld gives rise to a characteristic microstructure
consisting of grain boundary allotriomorphic ferrite, wedge-shaped parallel plates of
Widmanstätten ferrite, and the fine-grained bainitic phase termed acicular ferrite.
Microphases form later from the residual austenite.

While the essential theories of weld metal solidification are well understood, it
is still not possible to analytically predict the solidification structure, and hence the
distribution of solute in steel weld deposits. To enable this, research in this area
should aim to provide quantitative data on the rates of cooling experienced in the
initial stages of solidification, and, ideally, the problem should be approached both
experimentally and thermodynamically, to allow a complete formal description to
be developed.

Microstructurally, the model for the prediction of weld metal fusion zone has
been successful, however, more work on the nature of the acicular ferrite phase is
clearly desirable, since this phase in crucial for the design of high-strength high-
toughness low-alloy C-Mn weldments. Also, the enormous importance of inclusions
in influencing the microstructure and properties of low-alloy steel weld deposits
has, until recently, been underestimated, and much systematic work should be
addressed towards the understanding of their origin, and effects. An understanding
of the factors that control their size and spatial distribution would be particularly
welcome.

As regards the physical metallurgy of C-Mn weld deposits, there is much scope
for work to relate mechanical properties, in particular tensile strength, toughness,
and ductility, to the microstructure of both single-pass and multirun weld metals.
These themes are all developed in the work that follows.
REFERENCES


CHANGES IN SOLIDIFICATION MODE, AND THE MEASUREMENT OF COOLING RATES FOLLOWING SOLIDIFICATION DURING ARC WELDING

2.1 INTRODUCTION

The solidification process in a weld pool has been shown to have a considerable influence upon the properties of the resultant weld. It influences the development of microstructure (Edvardsson et al., 1976), and determines the distribution of alloying elements, and hence the homogeneity of the weld. Previous work on the cooling behaviour of welds (Garland and Kirkwood, 1974; Svensson et al., 1986) has tended to concentrate on the measurement and prediction of cooling rates for the temperature range 800-500°C, because these are important in determining the mechanism of austenite decomposition in the weld. This work, however, is concerned with cooling conditions and solidification processes at, and near, the melting temperature. The microsegregation that occurs during solidification is closely related to the size and morphology of the solidifying phase, the crystal structure of which in turn is dependent upon the cooling rate. For example, it is known that with fast cooling rates, low carbon steels may solidify directly as austenite, when δ-ferrite would be expected for cooling conditions closer to equilibrium (Edvardsson et al., 1976), since substitutional atom diffusion is slower in austenite, solidification with non-equilibrium austenite as the primary phase would profoundly influence the homogeneity of the weld deposit.

It would, therefore, be of great value to relate the primary solidification structure to the solidification parameters. Also, although a few pilot studies have been conducted (Kohno and Jones, 1978; Barlow, 1982) almost no quantitative data have been published giving information about the cooling rates at temperatures near the freezing temperature. However, work on the measurement of the thermal cycle experienced in the heat-affected zone (HAZ) during manual-metal-arc (MMA) welding (Baker, 1976) indicate cooling rates in MMA welding to be particularly fast relative to other welding processes.

The aim of this investigation was to develop, and utilize, a method of measuring
the rate of cooling at the solidification temperature encountered in the welding of low-alloy steels.

2.2 PRIMARY SOLIDIFICATION STRUCTURES

Although, solidification will not occur as austenite in the binary Fe-C system for an alloy containing less than 0.53 wt% C at equilibrium (see Figure 4.1), fast cooling rates can cause the primary solidification mode to be austenitic when ferritic solidification would normally be expected (Räsänen and Tenkula, 1972). In order to demonstrate that this could happen at relatively low carbon concentrations as a consequence of the fast cooling rates encountered in arc welding, two bead-on-plate welds were manufactured using specially-produced high-carbon electrodes.

For the first weld (Weld A), three parallel runs of an electrode with a nominal all-weld deposit composition of Fe-0.31C-1.46Mn-0.79Si wt% (Electrode A) were deposited onto a 20mm thick plate of (Swedish standard) SK1311 steel of nominal composition Fe-0.12C-0.55Mn-0.25Si wt%. A top bead was then deposited onto the buttered plate. The welding conditions were 120A/23V (D.C. +ve), and the welding speed was approximately 4mm/s. The second weld (Weld B) was fabricated under the same conditions, except that a consumable stick electrode of nominal deposit composition Fe-0.42C-1.56Mn-1.03Si wt% (Electrode B) was used. In this case, since the carbon content was particularly high, an additional layer, i.e. three runs, of buttering were applied to minimize dilution from the base plate, so that the carbon distribution in the top bead was homogeneous.

The compositions of the electrodes used, and the resultant welds are given in Tables 2.1 and 2.2 respectively.

<table>
<thead>
<tr>
<th>Electrode</th>
<th>Composition/wt%</th>
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<tbody>
<tr>
<td></td>
<td>C</td>
</tr>
<tr>
<td>A</td>
<td>0.31</td>
</tr>
<tr>
<td>B</td>
<td>0.42</td>
</tr>
</tbody>
</table>

Table 2.1: Welding rod deposit compositions
Weld Composition/wt%  
<table>
<thead>
<tr>
<th></th>
<th>C</th>
<th>Mn</th>
<th>Si</th>
<th>Cr</th>
<th>P</th>
<th>S</th>
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<tr>
<td>A</td>
<td>0.19</td>
<td>1.40</td>
<td>0.69</td>
<td>0.04</td>
<td>0.012</td>
<td>0.007</td>
</tr>
<tr>
<td>B</td>
<td>0.31</td>
<td>1.38</td>
<td>0.92</td>
<td>0.02</td>
<td>0.014</td>
<td>0.011</td>
</tr>
</tbody>
</table>

Table 2.2: Welds 2.1 and 2.2: compositions of top beads

Figures 2.1a and b show the microstructures of Welds A and B. Weld A solidified as δ-ferrite, and subsequently transformed to austenite. The micrograph shows the weld metal microstructure adjacent to the fusion boundary; large austenite grains, whose size is comparable to those of the base metal from which the primary microstructure grew epitaxially, can be seen, delineated by thin regions of discontinuous allotriomorphic ferrite. The location of the prior δ cell boundaries may be seen underlying the prior austenite microstructure, indirectly revealed by solute sensitive etching. It should be noted that this micrograph does not imply that the original δ columnar grains were not larger than the austenite grains, since each δ grain will have comprised many cells. It may be observed that the white cell boundaries do not stop at the prior austenite grain boundaries, meaning that the low carbon weld must have solidified as ferrite.

In Weld B, the solidification substructure does stop at the grain boundaries, indicating direct solidification as austenite. The strong contrast between individual cells is a consequence of the heavy microstructural segregation that is characteristic of an austenitic solidification process (Fredriksson and Stjerndahl, 1976). This behaviour is discussed in greater detail in Chapter 4. The almost complete absence of allotriomorphic ferrite, suppressed by the relatively high alloy content of the weld, should also be noted. The broad horizontal bands in the micrograph are due to solute banding, and correspond to periodic regions of solute enrichment or depletion. They occur as a natural consequence of fluctuations in the power of the arc causing periodic retentions in the advance of the weld pool interface (Davies and Garland, 1975).

In both micrographs, the primary phase is characterised by straight columnar grains, since they grew into a liquid phase, whereas the prior austenite grain

Figures 2.1a and b (overleaf): Microstructure of (a) Weld A, and (b) Weld B, showing solidification as primary ferrite and primary austenite respectively. Etchants: (a) 2% nitamyl followed by Klemm I tint etch; (b) 2% nital.
boundaries in Weld A (Figure 2.1a), which are the product of a solid state phase transformation, are irregular.

In summary, therefore, these results demonstrated that for the cooling rates typically found in manual-metal-arc welds, a 0.19 wt% C weld would solidify as ferrite, whereas a 0.31 wt% C weld would solidify as primary austenite. However, it was not known what cooling rates that the welds examined had actually experienced during solidification. It would be interesting to know this, since this would indicate how far the solidification process had been from equilibrium. Jernkontoret (1977) have reported that weld cooling rates vary during solidification between about 20 and 200°C. More accurate information than this, however, was not available, and this led to an enquiry as to how great the physical cooling rates actually were during welding. This is described in the next section.

2.3 EXPERIMENTAL METHOD

Following on from the above work, it was decided to attempt to measure the cooling rates that arise in the fusion zone during arc welding. Temperature measurement was to be carried out using a Pt/Pt-Rh thermocouple, protected by a cylindrical concrete shell. A number of attempts were made to see if pre-insertion of the electrode into the side of the weld would provide a suitable method for recording the temperature. Such a technique has been used in the past for recording the thermal cycles experienced in the HAZ during welding (Barlow, 1982). Unfortunately the high peak temperature encountered in arc welding ensured that the end of the thermocouple was destroyed in each case, (Figs. 2.2(a)-(d)), and the peak temperatures recorded were no more than ~1400°C, indicating that the new tip of the thermocouple was located within the HAZ. It was concluded that preposition-

Figures 2.2(a)-(d)) (overleaf): Cross-sections through welds containing sideways pre-inserted thermocouples mounted in bakelite. (Key to schematic diagrams: B = bakelite; BP = base-plate; T = thermocouple; W = weld metal). The micrographs show four single-pass bead-in-groove welds. In each case, a thermocouple has been drilled through the base-plate (on the right of the micrograph) to reach through to the weld. The thermocouples are observed to have received extensive damage as a consequence of the extremely high temperature of the welding arc. Remaining pieces of the thermocouples are arrowed. Etchant: swab-etched in aqueous NH₄S₂O₃.
ing of the thermocouple was unsuitable, although, this does not mean that such a technique could not ultimately be workable as a method for recording cooling rates in the fusion zone; however, harpooning into the weld pool, in which the thermocouple is inserted into the weld pool after the welding electrode has passed, seemed to be the best alternative.

A U-shaped groove of radius 5mm was machined onto 12mm thick SK1311 steel plate of nominal composition Fe-0.12C-0.55Mn-0.25Si wt%. OK 48,00 consumable electrode was deposited along this groove. On four occasions, a thermocouple was harpooned into the weld, and the change in temperature was recorded. The current and voltage used during welding were 180A and 22V respectively. Since welding can become very difficult if the current and voltage are changed, different cooling rates were achieved by manipulating the welding speed, \( v \), and the initial temperature of the base plate, \( T_0 \). Welding speeds and preheat temperatures for the four welds fabricated (designated Welds 2.1-2.4) are shown in Table 2.3.

<table>
<thead>
<tr>
<th>Weld ID.</th>
<th>( v/\text{mm/s} )</th>
<th>( T_0/\text{C} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>2.3</td>
<td>22</td>
</tr>
<tr>
<td>2.2</td>
<td>1.4</td>
<td>22</td>
</tr>
<tr>
<td>2.3</td>
<td>1.4</td>
<td>610</td>
</tr>
<tr>
<td>2.4</td>
<td>1.4</td>
<td>600</td>
</tr>
</tbody>
</table>

Table 2.3: Welding conditions for the cooling curve measurements.

A chart recorder was connected to the thermocouple to produce a permanent record of the change of temperature with time during welding.

One of the disadvantages of harpooning is that the exact position of the thermocouple in the centre of the weld cannot always be guaranteed (Kohno and Jones, 1978). However, Figures 2.3(a)-(d) show that the thermocouples were fairly centrally placed in the weld.

Figures 2.3(a)-(d) (overleaf): The micrographs show four single-pass welds in cross-section mounted in bakelite. (Key to schematic diagrams: B = bakelite; T = thermocouple; W = weld metal). A thermocouple within a concrete shell was harpooned into each weld immediately after welding. Note that the thermocouples
When the thermocouple is harpooned into the weld pool during welding, an increase in temperature is recorded. The thermocouple almost immediately becomes fixed to the underlying metal, and as the weld pool moves relative to the thermocouple, so the temperature decreases. With harpooning, the thermocouple does not experience the full severity of the arc, and accordingly, the tip of the thermocouple should not have been destroyed. Yet, in all four cases the recorded temperature did not exceed 1510°C. This is because a finite amount of time is required for the heat to overcome the thermal inertia of the thermocouple device, and to allow the heat to penetrate through the concrete shell to the thermocouple, during which time substantial cooling occurs in the rapidly-cooling weld deposit. However, the central positioning of the thermocouples indicated that the cooling curves that were recorded did represent the absolute cooling rates of the welds.

Figure 2.4 shows a schematic representation of a typical weld metal cooling curve, as was obtained in this research. By constructing tangents at 100°C intervals on the cooling curves obtained, it is possible to obtain the decrease in temperature with time. It should be mentioned that, at the peak temperature, the cooling rate is zero. However, this analysis is being applied at much lower temperatures, when the cooling rates are substantial. Table 2.2 shows how the cooling rate varied as a function of temperature in the four weld deposits. The cooling rate at 1350°C is given for weld 3, when the peak temperature recorded did not reach 1400°C. Sometimes the the curves were not truly smooth but fluctuated making some cooling rates uneven, and the calculated cooling rate correspondingly unreliable. This difficulty is denoted by parentheses.

will not appear continuous in these micrographs since they were inserted at an acute angle into the weld. The micrographs are merely intended to show the positions of the thermocouples within the welds. The variation in weld size arises because of the different welding conditions which were used in the four welds. Etchant: swab-etched in aqueous NH₄S₂O₃.
Figure 2.4: Schematic representation of cooling curve for a weld recorded near the solidification temperature. The initial instability prior to the peak temperature arises from the physical displacement of the thermocouple as it is inserted in the weld, exacerbated by the turbulent conditions within the weld pool itself.
<table>
<thead>
<tr>
<th>T/°C</th>
<th>Weld cooling rate/°C s⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2.1</td>
</tr>
<tr>
<td>1000</td>
<td>104</td>
</tr>
<tr>
<td>1100</td>
<td>157</td>
</tr>
<tr>
<td>1200</td>
<td>244</td>
</tr>
<tr>
<td>1300</td>
<td>314</td>
</tr>
<tr>
<td>1350</td>
<td>-</td>
</tr>
<tr>
<td>1400</td>
<td>342</td>
</tr>
</tbody>
</table>

Table 2.4: Cooling rate as a function of temperature for the four experimental welds.

It can be seen that between welds 2.1 and 2.4, the cooling rates resulting from the different process conditions vary by an order of magnitude. The weld metal was found to have a composition

Fe - 0.04C - 1.07Mn - 0.32Si - 0.05Ni - 0.04Cr - 0.1Cu - 0.016P - 0.016S wt%

Using a model due to Kirkaldy et al. (1978)† the alloy was predicted to have an equilibrium solidus temperature of 1515°C. In fact, this temperature will be depressed, since solidification temperature is a function of cooling rate (Fredriksson, 1976; Jernkontoret, 1977), but the temperature at which freezing was complete could be about 1500°.

Figures 2.5a-d plot the cooling rates experienced by the welds as a function of temperature. The simplest approximation which may be inferred from the experimental data would be that the cooling rate over a given temperature range is proportional to the temperature of the weld. In order to find the best fit lines, the hollow points in Figures 2.5b and d, whose validity was questionable, were given a relative weighting of 0.5. It is thus possible to estimate the cooling rates experienced by the weld at the point of solidification (taken to be 1500°) as follows:

- Weld 2.1: 422°C s⁻¹
- Weld 2.2: 153°C s⁻¹
- Weld 2.3: 104°C s⁻¹
- Weld 2.4: 56.5°C s⁻¹

† Discussed in detail in Chapter 4.
Figures 2.5a-d: Weld metal cooling rates as a function of temperature. (The hollow points are less accurate, and are given a half weighting).
2.4 ANALYSIS OF EXPERIMENTAL RESULTS

Figure 2.6 schematically shows the isotherms around the heat source in fusion welding. The shape of these isotherms can be predicted by considering the temperature distribution in a metal due to a moving point source. For a given heat source, moving at uniform velocity, a quasi-stationary temperature distribution will exist. So, if the arc moves along the $x$ coordinate as shown, the resulting heat distribution in a three dimensional solid plate is given by

$$\frac{d^2T}{dx^2} + \frac{d^2T}{dy^2} + \frac{d^2T}{dz^2} = 2kv \frac{dt}{d(x-vt)}$$  \hspace{1cm} (2.1)

where $k$ is the thermal conductivity of the metal being welded

$v$ is the velocity of the arc along the $x$ axis

and $t$ is the thickness of the plate being welded (Rosenthal, 1941; 1946).

The solution to this equation gives the temperature distribution about the moving heat source in the form of isotherms in the solid metal. The distance between isotherms in a given direction, $(x, y, z)$ is approximately given by

$$\lambda(x, y, z) \propto \frac{q}{kvt}$$  \hspace{1cm} (2.2)

where $q$ is the heat flux, or rate of heat input.

Subsequent models have attempted to take account of various welding variables, such as surface heat losses (Jhaveri et al., 1962), and the removal of latent heat (Ghent et al., 1979). Nevertheless, despite the various assumptions, Rosenthal’s equations have been found to give good agreement for isotherms around the heat source in welding, especially in the welding of thin sheet, when heat flow is largely two-dimensional (American Welding Society, 1976).

Depending upon whether heat flow in the weld can be regarded as three-dimensional downwards as well as lateral, the cooling rate of a weld metal at the centreline may be described by either thick or thin plate equations.
The thick plate equation, which considers three-dimensional heat flow from a point source states that the cooling rate

\[ R(T) = \frac{2\pi k}{H_{\text{net}}} (T - T_0)^2 \]  

(2.3)

where \( T \) is the temperature elevation above \( T_0 \), the initial temperature of the plate

and \( k \) is the thermal conductivity.

\( H_{\text{net}} \) is the weld heat input rate, often referred to simply as the heat input, and is related to the welding parameters thus

\[ H_{\text{net}} = \frac{q}{v} \]

\[ = \frac{UI}{v} \eta \]  

(2.4)

where \( U \) is the welding voltage, equal to 22V

\( I \) is the welding current, equal to 180A

and \( \eta \) is the coefficient of arc efficiency, taken as 0.775 for manual-metal-arc welding (Easterling, 1983).

The thin plate equation gives

\[ R(T) = 2\pi k \rho C \left( \frac{t}{H_{\text{net}}} \right)^2 (T - T_0)^3 \]  

(2.5)

where \( t \) is the plate thickness, equal to 12mm

and \( \rho C \) is the volumetric specific heat, equal to the product of the density of the material being welded, and its specific heat. For low-alloy steel, \( \rho = 7.87 \times 10^{-6} \text{kg} \)
mm$^{-3}$, and the specific heat of iron at, and close to, its freezing point, $C = 835$ J K$^{-1}$ kg$^{-1}$ (Touloukian and Ho, 1981).

To find which equation is appropriate, (i.e. whether thick plate or thin plate conditions prevail), the Adams' "relative plate thickness" criterion is applied. The relative plate thickness is a dimensionless quantity defined as (American Welding Society, 1976).

$$\tau = t \sqrt{\frac{\rho C(T - T_0)}{H_{net}}}$$

(2.6)

The thick plate equation applies when $\tau$ is greater than 0.9, and the thin plate equation when $\tau$ is less than 0.6. Values for the relative plate thicknesses of the four welds are given in Table 2.5 for $T = 1500^\circ$C.

<table>
<thead>
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<th>Weld</th>
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<tbody>
<tr>
<td>2.1</td>
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<tr>
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<td>0.62</td>
</tr>
<tr>
<td>2.4</td>
<td>0.62</td>
</tr>
</tbody>
</table>

Table 2.5: Relative plate thicknesses for Welds 1-4.

Therefore, from the values obtained, for Weld 2.1, the thick plate equation applies. For welds 2.2, 2.3 and 2.4, the thick plate equation should give a cooling rate which is too high, and the thin plate equation, one which is too low. $k(\delta$-Fe/1811K) has been taken as 0.039 W K$^{-1}$ mm$^{-1}$ (Touloukian and Ho, 1981)

Theoretical and measured values for the cooling rates of the four welds at 1495$^\circ$C are given in Table 2.6, and are plotted against one another in Figure 2.7.
Figure 2.7: Measured cooling rates for welds 1-4, compared against thick plate (▲) and thin plate (■) predictions. (For Weld 1, the thin plate equation was not applicable).
The experimental results provide quantitative data on the cooling rates encountered in weld deposits. The agreement of heat flow calculations with the experimental weld cooling rates is, in fact, better than expected, since the equations were not specifically developed from or for high temperature measurements. Also, the equations take no account of the finite size of the heat source, or of convection within the weld pool, and were not developed from high temperature measurements.

It is instructive to compare these results with those of Edvardsson (1975), who found in controlled directional solidification experiments, that an Fe-0.19C-1.47Mn-0.42Si wt% steel, cooled at 33°C/s, solidified as primary austenite. These results differ to those obtained in Weld 2.1, and suggest, therefore, that results obtained from directional solidification cannot readily be used to model weld pool solidification, perhaps because the influence of the base-plate on the solidification mode in welding needs to be taken into account.

### 2.5 SUMMARY

Solidification processes during manual-metal-arc welding have been studied, and observed changes in primary microstructure have been related to chemical composition and cooling conditions.

A cooling rate of approximately 600°C/s at the solidus temperature, estimated using empirical heat flow equations was found to result in solidification as δ-ferrite in a 0.19wt% C low-alloy C-Mn weld deposit, but to induce solidification in a 0.31 wt% C weld. This is a consequence of the high cooling rates which cause primary austenite precipitation, when under equilibrium conditions, δ-ferrite would be expected. The cooling rates experienced by manual-metal-arc welds at the point of solidification have been estimated for varying travel speeds and preheats.

<table>
<thead>
<tr>
<th>Cooling Rate/°C</th>
<th>Weld</th>
<th>2.1</th>
<th>2.2</th>
<th>2.3</th>
<th>2.4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measured</td>
<td></td>
<td>422</td>
<td>153</td>
<td>104</td>
<td>56.5</td>
</tr>
<tr>
<td>Thick plate</td>
<td></td>
<td>401</td>
<td>244</td>
<td>88.5</td>
<td>90.5</td>
</tr>
<tr>
<td>Thin plate</td>
<td></td>
<td>-</td>
<td>156</td>
<td>34.2</td>
<td>35.3</td>
</tr>
</tbody>
</table>

Table 2.6: Measured and calculated cooling rates at 1500°C
A method is described for measuring the cooling rates at, and near to, the solidification temperature of the weld pool by injecting a shielded thermocouple into the weld pool subsequent to the passage of the arc. Preinsertion of thermocouples was tried as a means by which the cooling rates during weld metal solidification could be measured. Unfortunately, conditions under the arc are so severe that the thermocouples there did not survive, and it is concluded that direct pre-insertion is not a viable means by which to measure \( \frac{dT}{dt} \) in a weld. That is not to say, however, that such a technique might not be practicable if modified.

Harpooning of the weld was more successful, with the temperature sensor being frozen into the weld pool during solidification. For a typical welding speed (2.3mm/s) the cooling rate in manual-metal-arc welding was found to be high, at over 400°C/s in the early stages of freezing. However, a reduction in travel speed and application of preheat have been found to reduce the rate of cooling substantially. Initial calculations show that measured cooling rates agreed with empirical thin-plate and thick-plate equations.

This work provides a preliminary basis for the quantitative prediction of the cooling rates experienced by welds during solidification.
REFERENCES


3.1 INTRODUCTION

In order to satisfy the ever increasing demand for improvements in the toughness of weld deposits in engineering structures, there is strong incentive to improve welding consumables and to design new welding methods (Abson and Pargeter, 1982). To do this systematically requires a method for modelling the microstructure and properties of welds as a function of its chemical composition, thermal history and many other variables.

The microstructure of a steel weld is complex; solidification involves the epitaxial growth of \( \delta \)-ferrite from the parent plate grains at the fusion boundary, and because of the high temperature gradients involved in arc welding it proceeds in a cellular manner. The resulting solid \( \delta \)-ferrite grains have an anisotropic columnar morphology. On further cooling, austenite forms in such a way that its final grain structure resembles closely the original \( \delta \)-ferrite morphology. However, if the carbon level or the substitutional alloy content or cooling rate is sufficiently high, then austenite is the first solid to form and columnar austenite grains grow directly from the melt. This is because of the small differences in the free energies of the two phases (Edvardsson et al., 1976). Whatever the mechanism of primary solidification, the austenite grains eventually undergo further transformation into a complex microstructure (described by Bhadeshia et al. (1985)) consisting of layers of allotriomorphic ferrite which decorate the austenite grain boundaries, Widmanstätten ferrite plates, intragranularly nucleated acicular ferrite plates and small amounts of martensite or degenerate pearlite. This is the “as-welded” microstructure, and it can have a profound influence on mechanical properties. For example, the layers of allotriomorphic ferrite are understood to be detrimental to toughness (Widgery, 1973; Ito et al., 1982; Tweed, 1982), whereas the morphology of acicular ferrite ensures that any crack has to follow a tortuous path during propagation thus imparting better toughness to the weld (Widgery, 1976; Ito et al., 1979, 1982).
A model now exists which is capable of estimating quantitatively the fusion zone of low-alloy steel welds, as a function of their chemical composition and welding conditions (Bhadeshia et al., 1985). The model does not however reveal any information about non-metallic inclusions which are inevitably present in welds. Inclusions in welds originate from oxides formed during weld deposition, or from the unintentional trapping of slag forming materials which are used to protect the molten metal during welding. Inclusions are known to initiate fracture in weld metals (Tweed and Knott, 1983; Schmidt-Van Der Burg et al., 1985; McRobie, 1985; Knott, 1985) so their content should be kept to a minimum. On the other hand, it is also believed that they are responsible for the intragranular nucleation of acicular ferrite (Ito and Nakanishi, 1976; Abson et al., 1979; Liu et al., 1982), a highly desirable phase from the point of view of toughness. In order to reach a compromise inclusion content with the right size distribution, it is essential that a method is developed for quantitatively predicting the important characteristics of inclusions in welds. For reasons which will become clear later, this work attempts specifically to establish whether inclusions in low-alloy steel weld deposits are distributed uniformly throughout the weld.

It has generally been assumed that the inclusions in are randomly distributed. However, a variety of evidence suggests that this may not be the case. Uhlmann et al. (1964), Cissé and Bolling (1971), Bolling and Cissé (1971), and others (Chernov et al., 1976; Pötschke, 1986), have shown (using organic and other solid-liquid-particle systems) that a moving interface can push some particles ahead of it while others are trapped passively by the advancing interface (Figure 3.1). For cellular solidification, the pushed particles can then locate themselves into crevices in the interface (e.g., cell boundaries) where they are subsequently enclosed by the solid, leading to a non-uniform distribution of inclusions, with larger particles decorating the cell boundaries.

Since the distribution of inclusions in the weld microstructure is determined during solidification when the inclusions are mobile in the melt, it seems possible that similar behaviour should occur during weld-metal solidification, which might provoke a non-uniform distribution of inclusions, perhaps to the columnar grain boundary sites where they would do most damage. For a steel solidifying as δ-ferrite, the preferential location of the inclusions at the columnar boundaries would be advantageous since the subsequent austenite transformation would cause the inclusions to finish up in or near the centre of the columnar austenite grain.
Figure 3.1: Pile up of zinc particles in thymol at the solid-liquid interface (taken at \( \times360 \)). (After Uhlmann, D. R., Chalmers, B., and Jackson, K. A. (1964), \textit{J. Appl. Phys.}, \textbf{35}, 2986-2993).
boundaries (Figure 3.2a). This is because the austenite grain boundaries would not coincide with the δ grain boundaries. Any inclusions at δ boundaries would not then be at the austenite boundaries (Akselsen et al., 1986). Also, the nucleation rate of acicular ferrite might be enhanced by the increased number of inclusions present in regions away from the austenite grain boundaries.

On the other hand, if solidification occurs with austenite as the primary phase, then there would be a non-uniform distribution of relatively large inclusions at the austenite grain boundaries (Figure 3.2b). In such circumstances, not only may the amount of acicular ferrite obtained in the final microstructure be reduced, but there would also be a concentration of inclusions in the weakest phase, allotriomorphic ferrite, which forms at the austenite grain boundaries. If inclusions enhance the grain boundary nucleation rate of allotriomorphic ferrite, then the situation would worsen since the volume fraction of undesirable allotriomorphic ferrite in the final microstructure would increase.

The aim of this particular work was to establish whether any preferential distribution of inclusions occurs during weld metal solidification, as a function of the solidification mode.

3.2 EXPERIMENTAL METHOD

In order to test for inclusion redistribution during solidification, four low-alloy steel manual-metal-arc welds were fabricated.

For one of the welds (Weld 3.1) a low carbon electrode was welded onto an 11mm thick, Fe–0.68C–1.02Mn–0.24Si–0.03P–0.03S wt% high carbon base plate using the bead-on-plate technique. According to the Fe–C equilibrium phase diagram, the high carbon concentration in the base plate will ensure that it is in the austenitic state before melting. In fact, solidification during welding is non-equilibriuous, but this can only stimulate further the tendency to form austenite rather than δ-ferrite. Furthermore, since grain growth at the fusion boundary is epitaxial, this would ensure austenitic solidification of the entire weld pool even though the deposit itself has a relatively low-carbon concentration. This is because there is far less nucleation occurring within the weld pool itself.

In order to study a weld which solidifies initially as δ-ferrite, a second weld
Figures 3.2a and b: Schematic diagram showing the location of inclusions in the microstructure of a weld for solidification as (a) δ-ferrite, and (b) austenite, assuming that the inclusions locate themselves preferentially at the cell boundaries during solidification. In Figure 3.2a the prior δ-ferrite boundaries and austenite boundaries diverge, since in arc welding the heat source is not stationary (Dadian, 1986).
(Weld 3.2) was deposited using an experimental medium carbon electrode. The electrode was clad onto a Fe-0.12C-0.55Mn wt.% base plate. Six runs, in a layer sequence 3-2-1 were used, so that dilution of the top bead, which was the bead examined, would be minimal. This procedure gave a medium carbon weld which solidified as \( \delta \)-ferrite.

For the third weld, weld 3.3, a normal low-carbon bead-on-plate weld was fabricated by welding a low-carbon electrode on a 20mm thick 0.14C-0.48Mn-0.32Si-0.028P-0.007S wt% base plate. Three buttering runs were carried out. Then, during welding of the fourth (top) bead, aluminium was added to the weld by feeding an aluminium wire into the weldpool, directly behind the arc. The effect of adding aluminium is to introduce a \( \gamma \)-loop (Figure 3.3), and thus to suppress the ferrite—austenite transformation. This would thus permit examination of the primary solidification microstructure at room temperature. Chemical analysis of the top bead of weld 3.3 proved extremely difficult because of the large amount of porosity which formed in the weld as a consequence of the aluminium, and, in fact, because some of the base plate may have been sampled in the analyses of the carbon and sulphur contents, the values obtained will be close, but not necessarily completely accurate. The amount of aluminium in the weld was estimated from a knowledge of the weight of aluminium wire consumed during welding of the final run to be \( \approx 5 \)wt%.

In all three cases, direct current (electrode positive) was employed, using a high current-low voltage (180A/23V) electric arc. The welding speed was approximately 4mm/s.

Finally, a 0.05C wt% MMA multipass arc weld was taken (Weld 3.4). This weld had been produced for use in experiments for the modelling of weld metal strength (Weld 5.2), and details of its fabrication are given in Section 5.2. The important point is that its manufacture was in no way unusual, and thus it could serve as a control specimen. Weld 3.4 was heat-treated at 600°C for 10 hours.

Weld metal analyses are given in Table 3.1.
Figure 3.3: Schematic diagram illustrating the effect of adding 5wt% Al to the iron-carbon equilibrium phase diagram, when a closed γ-field is introduced.
<table>
<thead>
<tr>
<th>Weld</th>
<th>Solidification Mode</th>
<th>Composition/wt%</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>C</td>
</tr>
<tr>
<td>3.1</td>
<td>Austenitic</td>
<td>0.29</td>
</tr>
<tr>
<td>3.2</td>
<td>Ferritic</td>
<td>0.19</td>
</tr>
<tr>
<td>3.3</td>
<td>Ferritic</td>
<td>0.12</td>
</tr>
<tr>
<td>3.4</td>
<td>Ferritic</td>
<td>0.10</td>
</tr>
</tbody>
</table>

* Not ascertained

Table 3.1: Weld metal analyses

The welds were sectioned, ground, and polished in oil prior to etching in order to avoid specimen pitting. A variety of different etchants were used in this work. Klemm I tint etch was found to produce the best results when made as follows: 660g Na$_2$S$_2$O$_3$.5H$_2$O was dissolved in 600ml of distilled H$_2$O at 40°C. Then, when etching, 1g K$_2$S$_2$O$_5$ (potassium metabisulphite) was added to 50cc of this base solution. Finally, the etchant was filtered before use. The scanning electron micrograph (Figure 3.10) was taken using a Cambridge Stereoscan S4 scanning electron microscope.

3.3 RESULTS

3.3.1 Weld 3.1: \( L \rightarrow \gamma + L \rightarrow \gamma \rightarrow \alpha + Fe_3C \)

Figure 3.4 shows weld 3.1 in cross-section, and illustrates the welding technique used. Figure 3.5 shows the microstructure of the weld from the base plate through to the top of the bead. The structural transition from columnar to cellular-dendritic growth may be seen.

In weld 3.1 the first phase to solidify was to be austenite. This was indicated by the large amount pearlite within the grains and the epitaxial growth at the fusion boundary, from a high carbon base plate whose structure at its melting point is austenite (Figure 3.6). The microstructure of the weld metal showed irregular grains of acicular ferrite, \((\alpha_a)\), and pearlite, (dark etch), bounded by thin layers of allotriomorphic ferrite, \((\alpha)\). Close to the fusion boundary, a substantial amount of Widmanstätten ferrite, \((\alpha_W)\), was also evident. The heat-affected base metal (Figure 3.7) was predominantly pearlitic, although large amounts of retained austenite, \((\gamma_{ret})\), and high carbon martensite \((\alpha'_{HC})\) were also present.
Figure 3.4: Cross-section macrograph of weld 3.1, illustrating the welding technique used. (Swab-etched in saturated aqueous NH$_4$S$_2$O$_3$).
Figure 3.5: Weld metal solidified as primary austenite (nominally 0.29C-0.76Mn-0.2Si). (Nitamyl (2\% v/v nitric acid in amyl alcohol), 10s, followed by Klemm I tint etch).
Figure 3.6: Weld 3.1: Microstructure at the fusion boundary for a weld solidifying as primary austenite. Note the curvature of the columnar grains due to the transient nature of the heat flow in the solidifying weld. (2% nital).

Figure 3.7: Weld 3.1: Micrograph of base plate near fusion boundary, showing high carbon martensite ($\alpha'^{HC}$) and a large amount of retained austenite ($\gamma_{ret}$). (Tint-etched with Klemm I).
It is known that during solidification the weld metal comprises a series of column-
nar grains growing inwards from the fusion boundary, each grain consisting of a
bundle of fine regular hexagonal cells all having approximately the same crystallo-
graphic orientation in space (Gretoft et al., 1986). This behaviour leads to regions
of microphases aligned along the cell boundaries, indicating a local difference in
chemical composition within the columnar grains, and Figure 3.8 shows this segre-
gation pattern. The cells within the grains only change orientation at the columnar
boundaries confirming that the weld solidified as austenite.

On etching the weld with picral, large inclusions were observed at the columnar
grain boundaries, (Figure 3.9).

Figure 3.10 is a scanning electron micrograph of the same weld etched in
bromine in methanol, which attacks the metal, but not inclusions (Hammar and
Svensson, 1977). It can be seen that there is a predominance of inclusions at the
prior austenite grain boundaries. Note that this technique is used simply to con-
firm the presence of inclusions at the boundaries, and is not generally applicable
since some inclusions may be washed away.

3.3.2 Weld 3.2: L→δ + L→δ + γ + L→γ →α + Fe₃C

The microstructure of weld 3.2 (Figure 3.11) was typical of that of a low-carbon
manganese steel weldment, and showed a columnar structure with layers of allotrio-
morphic ferrite at the prior austenite grain boundaries and fine plates of acicular
ferrite within the grains. Clusters of Widmanstätten ferrite plates can be seen at
the prior austenite grain boundaries.

Weld 2 solidified as δ-ferrite and subsequently transformed to columnar austen-
ite grains. The nature of the original δ-ferrite solidification structure was not
obvious, because the transformation to austenite during cooling destroys any mi-
crostructural evidence of the position of the δ–δ grain boundaries. It could however
be revealed by solute sensitive etching using Klemm I (Figure 3.12), which maps
the distribution of impurities in the microstructure; since these impurities segregate
during solidification to regions between the δ grains, the etch indirectly delineates
the positions of the prior δ boundaries. Inclusions were seen aligned along the prior
δ-boundaries.

It should be emphasized, however, that the inclusions were not aligned with
Figure 3.8: Weld 3.1: Epitaxial growth at the fusion boundary. The austenite solidification structure may be seen within the columnar grains. (2% nital).
Figure 3.9: Weld 3.1: Large inclusions are located predominantly at the grain boundaries of the solidifying phase (austenite).
Figure 3.10: Weld 3.1: Secondary electron image of deep-etched weld metal, showing inclusions (arrowed) at the columnar grain boundaries. (Deep-etched in 10% v/v bromine in methanol).
Figure 3.11: Weld 3.2: Weld metal microstructure. (Etchant: saturated aqueous ammonium persulphate).
Figure 3.12: Weld 3.2: Inclusions delineate the prior δ grain boundaries. (Nitamyl, followed by Klemm I tint etch).
the prior austenite grain boundaries. Recent work (Dadian, 1986) indicates that the δ/δ and γ/γ boundaries are neither coincident nor parallel under the influence of a moving heat source, as found in arc welding, but cross over each other, and this would account for the lack of alignment.

3.3.3 Weld 3.3: \( L \rightarrow \alpha + L \rightarrow \alpha \)

In weld 3.3, the addition of a small percentage of aluminium was sufficient to permit the weld to retain its ferritic solidification structure to room temperature to give a columnar microstructure of primary ferrite grains (Figure 3.13). Reaction of the aluminium with nitrogen from the atmosphere during welding to form aluminium nitrides gave the weld an extremely high hardness of over 700HV. The presence of aluminium also made the weld difficult to etch. However, on etching in acidified alcoholic copper (II) chloride, the solidification morphology of the δ grains was revealed, with the inclusions at the solidification boundaries (Figure 3.14).

3.3.4 Weld 3.4: \( L \rightarrow \delta + L \rightarrow \delta + \gamma + L \rightarrow \gamma \rightarrow \alpha + Fe_3C \)

As with weld 3.2, this weld solidified as ferrite, but the subsequent transformations to austenite, and then ferrite meant that any non-uniform inclusion distribution would be obscured by the microstructure that evolved. The microstructure of weld 3.4 is shown in Figure 3.15a, and shows the characteristic features of of any low-alloy C-Mn weld metal microstructure. A fine layer of allotriomorphic ferrite ornaments the grain boundaries. The carbon content (0.10C wt%) is slightly higher than is typical, and this led to a high volume fraction of acicular ferrite in the weld, at the expense of Widmanstätten ferrite, as expected (Evans, 1983). Tempering at 600°C had allowed the internal weld microstructure to recrystallize, although the original columnar grain boundaries were still present. This microstructure is shown in Figure 3.15b. Inclusions could be seen at and within the columnar grain boundaries, and aligned along their length. Experimental evidence has shown that the inclusion distribution of a weld is unaffected by subsequent heat treatment (Tweed and Knott, 1983). Thus, the inclusions observed were in the positions they were in when the weld had solidified as δ-ferrite. The work of Dadian (1986) has shown that for this to happen the inclusions would not necessarily have to be parallel to the prior austenite grain boundaries.
Figure 3.13: Microstructure of aluminium-containing weld. Small nuclei of austenite may be seen at the $\delta$-ferrite grain boundaries. (Picture: courtesy B. Gretoft, ESAB AB).
Figure 3.14: Weld 3.3: Micrograph of an aluminium-containing low-alloy steel weld. A uniform distribution of fine aluminium nitride particles comprises a key feature of the microstructure. Diagonally superimposed on this, inclusions can be seen aligned along the primary solidification boundaries. (Etchant: acidified alcoholic CuCl₂).
Figure 3.15: (a) As-deposited and (b) post-weld heat-treated, 600°C/10h. In Figure 3.15b, the inclusion distribution within the weld microstructure is revealed. The inclusions exhibit strong alignment (arrowed). (Etchant: 2% nital).
3.4 DISCUSSION

The size of the inclusions which locate themselves preferentially at the boundaries of the primary phase to solidify identifies them as primary indigenous inclusions, that is the deoxidation products of non-external origin which are present in the liquid during the freezing of the weld. They typically have dimensions ranging from 1 to 3μm for arc welding of the type considered here (Craig et al., 1979).

The nucleation, growth, and flotation of deoxidation products in liquid steel has been modelled by Turkdogan (Turkdogan, 1966), when the rate of nucleation in a weld is estimated by equating the number of nuclei to the number of inclusions found empirically. Knowing this, and the rate of growth of the inclusions, which is assumed to be limited by the diffusion of reactants to the surface of the inclusions, the rate of oxygen removal from the melt can be calculated. We find that for a weld metal, with a typical inclusion density of $10^7$ mm$^{-3}$, the inclusions should grow to almost their ultimate size in less than one second, implying that flotation is the critical process in determining the final inclusion and oxygen content of a weld.

Stokes' law states that the velocity of an ascending spherical inclusion,

$$v = 2gr^2\frac{(\rho_s - \rho_i)}{9\eta}$$

(3.1)

where $r$ is the radius of the sphere,

$\rho_s$ is the density of the steel,

$\rho_i$ is the density of the inclusion,

and $\eta$ is the coefficient of viscosity for the steel.

However, according to Stokes' law, if the weld pool is molten for, say, 5 seconds, the greatest distance travelled by, for example, a 1μm inclusion will be only be 1.7μm. Thus, Stokes' law cannot be a critical factor in the removal of small inclusions of the type considered here, although the suggestion that it does not control the deoxidation of welds is less certain for larger particles. As far as the present work is concerned, Stokes' law implies that the upwards flow of small inclu-
sions during solidification can be neglected. These conclusions concur with those of Grong et al. (1986), who studied the silicon-manganese deoxidation of mild and low-alloy steel weld metals. Weld pool conditions are extremely turbulent with temperatures beneath the arc exceeding perhaps 3000°C. This is especially true of arc welding, when electromagnetic stirring of the weld pool generated by Lorentz forces creates conditions of considerable turbulence within the pool (Woods and Milner, 1971). However, this turbulence ceases as the heat source recedes, and the temperature in the melt is reduced (Easterling, 1984). Grong et al. modelled deoxidation as a two stage process. Above about 1900°C continuous phase separation takes place as a consequence of turbulent flow conditions. In the cooler part of the weld pool, however, precipitated slag remains in the metal as finely dispersed particles. The solidification front during manual-metal-arc welding moves typically at a speed of 2mm.s⁻¹ (Easterling, 1983), whereas the small inclusions float at just 0.5μm.s⁻¹ so that the solidification front grows into a melt containing virtually stationary small particles.

The observed preferential location of inclusions at the boundaries between grains of the primary phase can be understood as follows. Inclusions in welds, being usually based on mixed (MnAl) silicates and oxides are assumed to exhibit a fully incoherent (high energy) interface with the liquid. Interfacial tension is highly sensitive to solute concentration, and the adsorption of surface active elements, such as oxygen or sulphur, reduces the interfacial tension in slag-metal systems. Thus, a gradient of concentration of surface active elements along an interface can result in a gradient of interfacial tension, and a concomitant interfacial flow. Such interfacial convection is usually called the “Marangoni effect” (Tinkler et al., 1984). This phenomenon, or some other force, perhaps surface tension, could explain the observed non-uniform distribution. Surface tension would tend to pull inclusions into the line of intersection between three grains. The solute-rich cell boundaries solidify at a lower temperature than the leading interface, and shrinkage during solidification, as well as the general motion of the interface, would tend to draw the inclusions in. The final structure would therefore contain more, and relatively larger particles, at the grain boundaries of the primary phase.

It should be noted that there are other possible mechanisms by which inclusions may end up preferentially at cusps in the solid-liquid interface, particularly if the interface can “push” inclusions in its direction of motion. Such an effect has been observed previously; Cissé and Bolling (1971), and Uhlmann et al. (1964) explained...
the observed pushing of particles by a solid–liquid interface in terms of a short range repulsive force between the particle and solid. However, work carried out by Weinberg (1984), in which the interaction of iron particles with a dendritic interface in a microgravity environment was studied, indicates that particles in a metal melt are not repelled by an advancing solid-liquid interface. Similarly, Schvezov and Weinberg (1985) carried out a series of modelling experiments, but found no evidence of particle interface repulsion. They considered that the Lifshitz-Van der Waals force might cause repulsion of a metal particle in a liquid metal, but, in fact, found it to be positive.

In another experiment, using nylon spheres for particles, and a lucite cellular surface as an interface, Schvezov and Weinberg found that the spheres pushed by the interface tended to locate themselves preferentially at to the cell boundaries as the interface advanced, rather than be trapped in the matrix. Whether particles can be pushed by the solid-liquid interface seems to depend on the particular system under consideration and it is not possible to be definitive about such an effect at this stage.

Whatever the mechanism leading to the non-uniform distribution of inclusions, it is evident that if austenite is the first phase to solidify, then numerous relatively large inclusions will be found at the austenite grain boundaries. This should have a very detrimental effect on toughness when allotriomorphic ferrite then forms at the austenite grain boundaries. It is emphasized that solidification mode will be austenitic either when the chemical composition at the fusion boundary is thermodynamically suitable to induce the epitaxial growth of austenite, or when the cooling rate and undercooling is high enough to kinetically favour austenite growth relative to that of δ-ferrite. The latter circumstance may arise with electron beam or laser beam welding and should be investigated in future work.

3.5 SUMMARY

Non-metallic inclusions in low-alloy steel welds have an important effect on the microstructure and properties of weld deposits. Work has been carried out in an attempt to understand the factors controlling the spatial distribution of such inclusions, with particular emphasis on the uniformity of the distribution, and the effect of solidification mode during MMA welding. The solidification mode has been controlled by using unusual combinations of base plates and experimental electrodes.
For the welding conditions used, the deposition of a low-carbon electrode on a high-carbon substrate caused the weld pool to solidify as austenite, whereas solidification proceeded with $\delta$-ferrite as the primary phase when a medium carbon electrode was deposited on a low-carbon substrate. This follows from the fact that weld pool solidification occurs by the epitaxial growth of grains at the fusion boundary, and it is the crystallographic structure of these which has determined the solidification mode. The addition of aluminium to the weldpool was found to suppress the $\delta \rightarrow \gamma$ phase transformation, and allowed cooling of the weld without a subsequent phase transformation.

It has been found in four separate experiments found that inclusions in low-alloy steel welds deposited by a MMA technique are not uniformly distributed; they tend to locate themselves preferentially to the boundaries of the first phase to solidify. For an austenitic solidification mode, the inclusions are mostly located at the austenite grain boundaries and hence are present in the allotriomorphic ferrite which forms from the austenite at the grain boundaries. For solidification as $\delta$-ferrite, the subsequent transformation to austenite ensures that most of the inclusions in the final weld are located away from the austenite grain boundaries, in regions where they can contribute towards the intragranular nucleation of acicular ferrite. This behaviour dictates that welds which solidify as austenite (either because of a high-carbon substrate or because the welding process leads to a high cooling rate during solidification) should have relatively poor toughness.

The reason for the observed non-uniform distribution of inclusions can be attributed tentatively to surface tension effects at the solidification front (Marangoni effect) or to the pushing of inclusions by the solid–liquid interface.
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CHAPTER 4

THERMODYNAMIC PREDICTION OF
THE LIQUIDUS, SOLIDUS, AND AE3 TEMPERATURES, AND
PHASE COMPOSITIONS FOR LOW-ALLOY MULTICOMPONENT STEELS

4.1 INTRODUCTION

The vast majority of steel weld deposits solidify under highly nonequilibrium cooling conditions. A consequence of this is the chemical segregation of substitutional alloying elements during solidification, a segregation that persists as the weld cools to ambient temperature. Solidification-induced segregation of interstitials is usually not a problem due to the ease with which they can diffuse and homogenize during cooling. The presence of substitutional element segregation can greatly influence the subsequent transformation of austenite into ferrite with reaction kinetics in general being accelerated in the solute-depleted regions. The formation of ferrite in these regions causes a redistribution of carbon into the remaining austenite whose hardenability is therefore increased. It has been demonstrated that such effects can have a major influence on the development of microstructure (Gretoft et al., 1986), and any method for alloy design must take them into proper consideration.

Weld metal compositions typically solidify as delta-ferrite ($\delta$), and subsequently transform to austenite ($\gamma$), and then to ferrite ($\alpha$). In order to obtain a general model for the prediction of the properties of a weld metal, it will be necessary to be able to predict the chemical segregation behaviour during solidification. For low-alloy C-Mn steel weld deposits solidifying as $\delta$-ferrite, the solute-enriched prior $\delta$-boundaries will finish up approximately within the centre of the austenite grains. The effect of the segregation will be to raise the temperature at which allotriomorphic ferrite first forms, and to increase the temperature range over which, $\alpha$ forms. Hence, the ultimate volume fraction for a given set of cooling conditions will increase (Strangwood and Bhadeshia, 1987). Conversely, for solidification as austenite, since regions in the proximity of the austenite boundaries would be solute-enriched, nucleation of $\alpha$ would be expected to be more difficult (Gretoft et al., 1986). To predict weld metal segregation quantitatively will necessarily require a knowledge of the solidification temperature, solidification range, degree of parti-
tioning in the melt, and partition coefficients for the carbon and solute elements in the steel. This work is an attempt at modelling the high temperature region of the phase diagram for multicomponent steels using the general thermodynamic techniques developed by Kirkaldy and co-workers (Baganis and Kirkaldy, 1978; Kirkaldy, 1978). In order to check the consistency of the calculations, and of the thermodynamic data used, calculations were also attempted for the $\alpha/\gamma$ equilibria, where the amount of experimental data available as a check of theory is far greater.

4.2 THE SOLIDIFICATION OF STEEL

The solidification of steel can take place in three ways:

- primary ferrite formation;
- primary ferrite formation followed by a peritectic reaction;
- primary austenite formation

For most low-alloy steel weldments, solidification entails a peritectic transformation (Figure 4.1). In plain carbon steels, the high diffusivity of carbon at the peritectic temperature means that the peritectic reaction is very rapid, and all of the primary dendrites transform to the more stable austenite. However, quenching specimens from $\gamma/\delta + L$ field has shown there to be considerable residual melt between solidified dendrites, and, in some steels, evidence of this may be seen in the completely solidified structure (Erokin et al., 1960). At higher carbon contents, the primary crystals are $\delta$, but just below 1500°C, a peritectic reaction takes place, and the remainder of the weld solidifies as austenite.

The mechanism of solidification, and in particular the peritectic reaction, in iron-base alloys has been investigated most recently by Fredriksson and his co-workers using unidirectionally solidified steels (Fredriksson, 1976; Fredriksson and Stjerndahl, 1982). Metallographic and microprobe analysis of quenched samples allowed the solidification process to be analysed. It was found that ferrite-stabilizing elements can segregate strongly to the ferrite during solidification. Austenite-stabilizing elements favour a peritectic reaction during the solidification process and ferrite-stabilizing elements favour a eutectic reaction (Fredriksson, 1977). Experimental and theoretical work (Sterenbogen et al., 1976; 1977) indicates that the greatest influence on the mode of solidification and the dimensions of the two phase region in the welding of steel is that exerted by carbon whose concentration must
Figure 4.1: Peritectic region of the Fe-C phase diagram. (After "Binary Alloy Phase Diagrams", Ed., T. B. Massalski, American Society for Metals, Ohio 44073, Vol. 1, 563).
therefore be known the most accurately. The carbon content largely controls the constitutional supercooling of the system. The peritectic reaction is influenced by the diffusion rate of the different alloying elements in austenite as well as in ferrite. This in turn will influence segregation behaviour. For a fixed carbon content, adding an alloying element will either expand or contract the $\gamma$-field, too. Most iron-base alloys contain one or more austenite-stabilizing elements (e.g. C, Ni, Mn) and one or more ferrite-stabilizing elements (e.g. P, Cr, Mo).

The segregation behaviour of an alloying element can be characterised using the segregation ratio $S$, defined as the local maximum in alloy content divided by the local minimum. The calculation of the segregation ratio for primary precipitation of ferrite as been made by Fredriksson and Stjerndahl (1982), the major assumptions being negligible undercooling from radius of curvature effects, no macrosegregation, complete diffusion in the liquid in interdendritic spaces, and equilibrium in the liquid at the solid-liquid interface. It is assumed (Fredriksson, 1976; Fredriksson, 1977) that the lever rule describes the solidification process during primary precipitation of ferrite. Let $C_s(t)$ be the solute concentration at the solid-liquid interface. Then, by using a mathematical model derived from homogenization of a cast structure (Kattamis and Flemings, 1965; Purdy and Kirkaldy, 1971), the concentration distribution as a function of time can be described by the relation

$$C(x, t) = C_s(t) - (C_s(t) - C_0k) \exp \frac{-\pi^2}{\lambda^2}Dt \sin \frac{\pi x}{\lambda}$$  \quad (4.1)

$t$ is the holding time

and $x$ is the distance from $x = 0$ to $x = \lambda$.

The symbols used are defined in Figure 4.2. At the end of the solidification process the concentration distribution is sinusoidal, the wavelength being twice the distance between the primary plates. In this case, since the diffusion rate in ferrite is rather high, the largest possible wavelength is chosen. Then, $C_s$ is given by the following material balance

$$C_0 \cdot \lambda = C_0 \int_0^\lambda (C_s(t) + (C_s(t) - C_0k)) \exp \frac{-D\pi^2t}{\lambda^2} \sin \frac{\pi x}{\lambda} \, dx$$ \quad (4.2)

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Figure 4.2: Theoretical distribution of alloying elements for calculations of segregation ratio. (After H. Fredriksson and J. Stjerndahl (1982), Met. Sci., 16, (12), 577).
which gives

\[ C_s(t) = C_o \cdot \frac{1 - \left[ (2k \exp - \frac{D\pi^2 t}{\lambda^2} )/\pi \right]}{\left( 1 - \frac{2}{\pi} \exp - \frac{D\pi^2 t}{\lambda^2} \right)} \]  

Using Eqns. 4.1 and 4.3, the segregation ratio becomes

\[ S = \frac{1}{\left\{ 1 - \left[ 1 - k(1 - \frac{2}{\pi} \exp - \frac{D\pi^2 t}{\lambda^2}) \right] \exp - \frac{D\pi t}{\lambda^3} \right\}} \]  

To calculate the segregation ratio one must know the solidification time and the dendrite plate space. However, if one assumes a constant cooling rate, they can be related thus:

\[ t = \Delta T / \left( \frac{dT}{dt} \right) \]  

and \[ \lambda = A \left( \frac{dT}{dt} \right)^n \]

where \( \Delta T \) is the solidification range, and \( A \) and \( n \) are experimentally determined constants. Substituting in Eqn. 4.4 then gives

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For primary precipitation as austenite, segregation behaviour can be calculated approximately starting from the modified Scheil equation first derived by Flemings et al. (1966) to give

\[
S = \frac{1 - k(1 - \frac{2}{\pi} \exp - \frac{\pi^2 D \Delta T}{A^2 \left(\frac{dT}{dt}\right)^{1+2n}})}{1 - \frac{2k}{\pi} \exp - \frac{\pi^2 D \Delta T}{A^2 \left(\frac{dT}{dt}\right)^{1+2n}}} \exp - \frac{\pi^2 D \Delta T}{A^2 \left(\frac{dT}{dt}\right)^{1+2n}}
\]

(4.7)

Thus, it can be seen that, in both cases, for a constant cooling rate, the amount of segregation experienced in steels for solidification as either ferrite or austenite can be directly related to the solidification range of the alloy and the partition ratios of the solute elements.

4.3 METHOD OF ANALYSIS

One of the most important factors which needs to be considered in the thermodynamic modelling of the Fe-C-X multicomponent system is that it ceases to retain the characteristics of infinite dilution for concentrations above about 0.2 wt%C (Darken and Gurry, 1953; Schürmann et al., 1987). In the analysis of Baganis and Kirkaldy (1978), which is used in the present work, this problem is circumvented by determining the temperature deviation of a particular phase boundary from the corresponding boundary in the binary Fe-C system. The change in carbon concentration at a phase boundary, due to the addition of substitutional alloying elements, is given by summing the effects due to each individual element. The large amount of thermodynamic data on Fe-X and Fe-C-X systems that has been accumulated over the last 20 years makes it possible to carry out these thermodynamic calculations with high accuracy.
In the following description, Fe is designated as zero, C as 1, and the alloying elements Si, Mn, Ni, Cr, Mo, Cu, V, Nb, Co, W as \(i(=2\) to \(n\)) respectively. The mole fractions in each phase are designated as \(X_i(i=0\) to \(n\)). A general temperature coordinate system on a phase boundary in the pure Fe-C system is designated \(T_0\). The temperature deviation from \(T_0\) due to the addition of substitutional alloying elements, \(\Delta T\), is calculated for the required range of \(T_0\), so that the phase boundary, \(T\{Fe-C-X(i)\}\), may be found. This procedure follows the classical “depression of the freezing point” relation due to Van’t Hoff [see Darken and Gurry (1953), 222-224]. In multicomponent alloys, the temperature changes due to individual alloy additions, are additive, so long as solute-solute interactions are taken as negligible. The interactions between elements in solution are represented by \(\epsilon_{ik}\) are empirical coefficients known as the Wagner interaction parameters, and the above assumption of additive \(\Delta T\) values is the same as saying that the interaction between elements \(i\) and \(k\), \(\epsilon_{ik}(i \neq k, i \text{ and } k > 1) = 0\). In fact, this is not strictly correct (Kagawa et al., 1985), and silicon, especially, can interact with other solute elements (Craska and McLellan, 1971). However, Kirkaldy and his co-workers found that this assumption is valid so long as the total alloying element content is less than about 6wt% and the silicon content is less than 1wt%.

In order to calculate the temperature deviation at a phase boundary, \(\Delta T\), Baganis and Kirkaldy (1978) started with the relationship for the equality of the chemical potentials in the two phases which are in equilibrium. For example, for the austenite + liquid/liquid phase boundary, for Fe

\[
X_0^\gamma \gamma_0 = X_0^L \gamma_0 \exp \left( \frac{\Delta^o G_0^{\gamma-L}}{RT} \right)
\]

where \(X_0 = 1 - \sum X_i^1\), is the mole fraction of iron, and \(\gamma_0\) is the activity coefficient for the iron for which the superscripts \(\gamma\) and \(L\) denote the austenite and liquid phases respectively.

\(\Delta^o G^{\gamma-L} = G_L - G_\gamma\), or, more generally, the difference between the Gibbs free energies of the pure higher and lower temperature phases.

and \(T\) is the phase boundary temperature.
Similarly for \( C(n = 1) \) or component \( i \)

\[
X_i^\gamma \gamma_i^\gamma = X_i^L \gamma_i^L \exp \left( \frac{\Delta^o G_i^{\gamma-L}}{RT} \right) \tag{4.10}
\]

The Wagner-Taylor expansions for the activity coefficients (Wagner, 1952) were then substituted into Eqns. 4.10 and 4.11. Eventually, this gave the temperature deviation in the form

\[
\Delta T = RT_0^2 \sum_{i=2}^{n} A_i X_i^L \tag{4.11}
\]

where \( X_i^L \) is the mole fraction of component \( i \),

and where

\[
A_i = \frac{A_i^\circ - \{(1 + X_i^L(1 - X_i^L)(\epsilon_{11}^i - \epsilon_{11}^\gamma A_i^\gamma))^\circ \exp \{ \frac{\Delta^o G_i^\circ}{RT_i^2} - \frac{X_i^L}{2} (\epsilon_{11}^i - \epsilon_{11}^\gamma A_i^\gamma) \} \}}{X_i^L \Delta^o H_i A_i^\circ + (1 - X_i^L) \Delta^o H_0 \exp \{ \frac{\Delta^o G_i^\circ}{RT_i^2} - \frac{X_i^L}{2} (\epsilon_{11}^i - \epsilon_{11}^\gamma A_i^\gamma) \}}
\]

for which

\[
A_i^\circ = \frac{\exp \{ \frac{\Delta^o G_i^\circ}{RT_i^2} + \epsilon_{1n}^L X_i^L \}}{1 + \epsilon_{1n}^\gamma X_i^L \exp \{ \frac{\Delta^o G_i^\circ}{RT_i^2} \}}
\]

where \( n = 1 \) or \( i \) (Kirkaldy et al., 1978).
\( \Delta^o H_0 \) and \( \Delta^o H_1 \) are the standard molar enthalpy changes corresponding to \( \Delta^o G_0 \) and \( \Delta^o G_1 \) respectively.

This was the relationship used for the determination of the Fe-C-X(i) multi-component equilibrium phase diagram. The solute elements for which the program has been written are those that might commonly be found in low-alloy steels, (Mn, Si, Ni, Cr, Mo, and Cu), although, if the relevant free energy changes per unit of solute dissolving (\( \Delta^o G \)) and the interaction parameters (\( \epsilon \)) are known, \( \Delta T \) can in principle be calculated for any alloy.

4.4 PREDICTION OF AE3 TEMPERATURE

The overall intention of this and other current research is to be able to predict the mechanical properties of multipass welds. This requires a detailed knowledge of the thermal history of the weld, and necessarily the transformation temperatures of the steels. In welding, the AE3 temperature which has a considerable influence on, inter alia, the relative volume fractions of the phases present in the as-welded microstructure, and the size of the reaustenitised region in multipass welds. Therefore, as a first step, a program was written to allow the AE3 temperature to be predicted, using the method described. A series of modifications were incorporated into it as follows:

- The program had been used for Mn, Si, Ni, Cr, Mo and Cu additions (Baganis and Kirkaldy, 1978). In addition, the elements for Nb, Co, V, and W were included, using further data given by Kirkaldy et al. (1978).

- AE3 values for \( T_0 \) were formulated into a subroutine using accurate values derived from equations due to Bhadeshia and Edmonds (1980) giving \( T_0 \) down to 200°C. Extrapolating the AE3 in this manner would be potentially very useful, allowing, for example, growth rate kinetics to be calculated at temperatures well below the eutectoid temperature (Bhadeshia, 1985a).

- Although, data were provided for values for the standard Gibbs free energy change accompanying the \( \alpha/\gamma \) transformation in pure iron (Harvig, 1978), \( \Delta^o G_{\alpha\rightarrow\gamma} \), since a long-term aim was to extrapolate the AE3 to lower temperatures, the data due to Kaufman et al. (1963), which gives values down to 0K, and which are known to be reliable over the entire temperature range of
interest (Bhadeshia, 1985b) were used. $\Delta^oG^\alpha_{\gamma}^-$ was represented by curve-fitting values from Table 3 of Kaufman et al. (1963), and later corrected values for $\Delta^oG^\alpha_{\gamma}^-(T > 1183)$ from Kaufman and Bernstein (1970).

- Values for $\Delta^oH^\alpha_{\gamma}^-$ were obtained from work due to Kaufman et al. (1963). For temperatures below 1183K, the tabulated data were interpolated using cubic splines (Hayes, 1974).

In applying Eqn. 4.11 to the calculation of the $Ae_3$, Baganis and Kirkaldy (1978) had taken $\varepsilon_{11}$ as taken zero. They argued that the error introduced is negligible, since the interaction parameter is multiplied only by the very low concentration of carbon in ferrite. This assumption can be assessed quantitatively. Figure 4.3 shows the carbon sublattice in a crystal of $\alpha$-Fe. The b.c.c. unit cell contains two iron atoms and six carbon sites. (This ignores tetrahedral sites, but the probability of their occupation is rather low). From Figure 4.1, the maximum solubility of carbon in $\delta$-iron is 0.09 wt% = 0.417 at%. Therefore, there are $(99.6/0.417) = 239$ iron atoms for every carbon atom, or there is one carbon atom for every 119 unit cells, so that, even at saturation, the probability of two carbon atoms even being in the same unit cell is only 0.004. Thus, their assumption seems justified and was adopted.

Since all the thermodynamic functions used were dependent on temperature, $\Delta T$ cannot be obtained from a single application of Eqn. 4.11, but has to be deduced iteratively. For this purpose, a loop was included in the program. Initially, $T$ was set as $T_0$, and a trial value of $\Delta T$ was calculated. Then, the program was rerun with $T = (T + \Delta T)$. This procedure being repeated until the value of $T$ changed by less than 1° in successive iterations (typically 5 times). A listout of the program is given in Appendix 1. Results for all the alloying elements were drawn up and checked for correspondence with data from Fe-X binary phase diagrams compiled by Kubaschewski (1982), and overall agreement was excellent. However, discrepancies were observed with the Fe-Mn, Fe-Ni, and Fe-Nb systems, and these are discussed here.

- **Fe-Mn**: As Baganis and Kirkaldy (1978) also found, a systematic discrepancy was observed between experimental and calculated values for the Fe-Mn system, attributable to errors in $\Delta^oG_{\text{Mn}}^\alpha_{\gamma}^-$. Instead, data were used due to Gilmour et al. (1972), who calculated $\Delta^oG_{\text{Mn}}^\alpha_{\gamma}^-$ between 700 and 850°C using experimental
Figure 4.3: Location of the octahedral interstices [●] in a b.c.c. crystal. (After Cohen, M. (1962), *Trans. AIME*, 224, 645).
results on the Fe-C-Mn system. In their work, $\Delta^\circ G_{\text{Mn}}^{\alpha-\gamma}$ was found as a function of temperature from a knowledge of the activities, and molar concentrations, of manganese in austenite and ferrite at equilibrium to give

$$\Delta^\circ G_{\text{Mn}}^{\alpha-\gamma} = 25.57T/K - 32640 \text{ J/mol} \quad (4.12)$$

- **Fe-Ni:** Kirkaldy *et al.* (1978) postulated that errors in predicting the Ae3 at lower carbon contents (higher temperatures) might be due in part to an error in $\Delta^\circ G_{\text{Ni}}^{\alpha-\gamma}$. Sharma and Kirkaldy (1973), whose data had been used by Kirkaldy *et al.* (1978), give

$$\Delta^\circ G_{\text{Ni}}^{\alpha-\gamma} = -1.90 \times 10^4 + 13.5T \text{ J/mol} \quad (4.13)$$

A new value for $\Delta^\circ G_{\text{Ni}}^{\alpha-\gamma}$ was calculated for the present work using the value for $\Delta^\circ G_{\text{Ni}}^{\gamma-L}$ given by Uhrenius. (Uhrenius, 1978). Thus, since these quantities are additive

$$\Delta^\circ G_{\text{Ni}}^{\alpha-\gamma} = \Delta^\circ G_{\text{Ni}}^{\alpha-L} - \Delta^\circ G_{\text{Ni}}^{\gamma-L}$$

$$\Delta^\circ G_{\text{Ni}}^{\alpha-L} = 8.88 \times 10^4 - 1.59T \text{ J/mol} \quad \text{(Kirkaldy *et al.*, 1978)}$$

$$\Delta^\circ G_{\text{Ni}}^{\gamma-L} = 1.46 \times 10^4 \text{ J/mol (Uhrenius, 1978)}$$

which gives

$$\Delta^\circ G_{\text{Ni}}^{\alpha-\gamma} \approx -2.35 \times 10^4 - 1.6T \text{ J/mol} \quad (4.14)$$

These changes made for a substantial improvement in the description of the Fe-Ni system.

- **Fe-Nb:** A large deviation from the $\alpha/\gamma$ phase boundary was found due to an error in $\Delta^\circ G_{\text{Nb}}^{\alpha-\gamma}$. Kirkaldy *et al.* (1978) give

$$\Delta^\circ G_{\text{Nb}}^{\alpha-\gamma} = 60.0 - 5.4 \times 10^{-3}T \text{ J/mol} \quad (4.15)$$
Figures 4.4a and b: Pseudo-binary phase diagrams illustrate the effect on the $Ae_3$ temperature of adding 0.5 wt% of a) manganese and b) silicon to binary iron-carbon.
Figure 4.5: Comparison of predicted and measured values for the $Ae_3$ temperature for a variety of steels.
Figure 4.6: Experimental and calculated values for the Ae₃, using experimental data due to Grange (1961).
the standard error being less than ±10°C. Data were also taken from Grange (1961) consisting of an analysis of nineteen medium carbon low-alloy steels of commercial purity. Grange identified the $A_{e3}$ temperature as the temperature at which the last trace of ferrite transformed to austenite on prolonged isothermal heating. This work, as with dilatometry on heating, would tend to yield higher than true equilibrium values. This concurs with the results obtained in Figure 4.6, the mean apparent overshoot of the experimental results obtained being approximately 8°C.

4.5 PREDICTION OF PERITECTIC REGION

4.5.1 Liquidus Temperature

Over recent years it has become apparent that the mode of solidification is a determining factor in the subsequent development of the weld metal microstructure (Watanabe, 1975; Cochrane, 1983). However, to attempt to model the former would require a knowledge of the steel’s solidification behaviour. Although, Eqn. 4.11 had been applied widely to the prediction of the $A_{e3}$ temperature, the accuracy of the equation at predicting the liquidus and other peritectic temperatures of low-alloy multicomponent steels does not seem to have been verified. Kirkaldy and Baganis did compute the peritectic part of the phase diagram for several ternary alloys, but their calculations do not appear to have been compared against experimental data.

At the outset of this work, an attempt was made to avoid some of the mathematical assumptions made by Kirkaldy et al. (1978) in deriving Eqn. 4.11, [see Appendix I of Kirkaldy et al.(1978)]. To do this, the three equations which had been combined to derive Eqn. 4.11 were solved individually. The first two equations quantitatively define $X_i^\gamma$ and $X_i^L$ ($i = 2\rightarrow 11$) as a function of alloy content, thus

$$X_1^\gamma \exp(\varepsilon_{11}^\gamma X_1^\gamma) = X_1^L \exp\left(\frac{\Delta^o G_1}{RT_o} - \frac{\Delta^o H_i \Delta T}{RT_o (T_o + \Delta T)} + \varepsilon_{11}^L X_1^L\right)$$ (4.18)

and

$$X_i^\gamma \exp(\varepsilon_{ii}^\gamma X_i^\gamma) = X_i^L \exp\left\{\frac{\Delta^o G_i}{RT_o} + \varepsilon_{ii}^L X_i^L\right\}$$ (4.19)

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Then, the deviation from the Fe-C liquidus boundary, $\Delta T$, is obtained by solving for $X_i^\gamma$ and $X_i^L$, and substituting into Eqn. 4.20:

$$\frac{\Delta^\circ G_o}{RT_o} - \frac{\Delta^\circ H_o \Delta T}{RT_o(T + \Delta T)}$$

$$- \ln|1 - X_i^\gamma - \sum_{i=2}^n X_i^\gamma| + \ln|1 - X_i^L - \sum_{i=2}^n X_i^L|$$

$$+ \frac{\epsilon_{11}^\gamma}{2} (X_1^\gamma)^2 - X_1^\gamma \sum_{i=2}^n \epsilon_{11}^\gamma X_i^\gamma + \frac{\epsilon_{11}^L}{2} (X_1^L)^2 - X_1^L \sum_{i=2}^n \epsilon_{11}^L X_i^L = 0 \quad (4.20)$$

In fact, it was soon found that these equations gave almost the same answers as those calculated using Eqn. 4.11, and because this method was much more complicated, it was abandoned.

Most of the data required were already found in Kirkaldy et al. (1978). However, several phase boundaries on the binary phase diagram were not included in that analysis; these were the ferrite and austenite solidus, and the $\delta/\delta + \gamma$ line. Also, the equation given in Kirkaldy et al. (1978) for $T_o$ for the austenite liquidus as a function of carbon due to Benz and Elliott (1961) did not appear to match the data in Kirkaldy et al. (1978) contain the following errata:

1. $\Delta^\circ G_{Mn}^{\alpha-\gamma} = -26650 + 42.69T - 0.017T^2$ cal/mol, not $0.17T^2$.
2. $\Delta^\circ G_{Mn}^{\gamma-\delta} = 430 - 0.305T$ cal/mol, not 650.
3. $\Delta^\circ G_{Mn}^{\alpha-\gamma} = 3500 - 2.308T$ cal/mol, not 3100.
4. Table III should be headed $\Delta^\circ G_i^{\gamma-L}$, not $\Delta G_i^{\alpha-L}$.
5. $\Delta^\circ H_i^{\gamma-L} = -5360$ cal/mol, not $-5630$.
6. $T_o^{\gamma-\gamma+\alpha} = 1185 - 150.3$ wt\%C + 216(0.865 wt\%C)^4.26 K, not 1115.

Equation 1, and in Appendix I, Eqns. 2, 14, 17, 18, 21, and 22 are also published incorrectly, and the reader is referred to this text, and to Baganis and Kirkaldy (1978). In addition, in Tables I, II, and III, the standard state superscripts are omitted.

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published A.S.M. data (Figure 4.1), and a new curve was calculated. From the Fe-C equilibrium phase diagram the lines were respectively calculated to be

\[ T_0^\delta \rightarrow \gamma + L = 1809 - 201.3(\text{wt}\%\text{C}) K - 2949(\text{wt}\%\text{C}) K \] (4.21a)

\[ T_0^\gamma \rightarrow \gamma + L = 1793 - 146.7(\text{wt}\%\text{C}) - 16.74(\text{wt}\%\text{C})^2 K \] (4.21b)

\[ T_0^{\gamma + \delta} = 1666 + 1122(\text{wt}\%\text{C}) K \] (4.21c)

and

\[ T_0^{\gamma + L \rightarrow L} = 1783 - 164.0(\text{wt}\%\text{C}) - 7.869(\text{wt}\%\text{C})^2 K \] (4.21d)

In order to find out if any data values were suspect, the carbon contents, \( x_f \), was set to zero so that dilute binary phase diagrams were generated for each element. In this way \( \Delta T \) for each solute element could be checked. Although, general agreement was excellent, a systematic discrepancy was found for the Fe-Mn system, and in this work \( \Delta^\circ G_{Mn}^{\gamma \rightarrow L} \) has been estimated from values for \( \Delta^\circ G_{Mn}^{\delta \rightarrow \gamma} \) and \( \Delta^\circ G_{Mn}^{\gamma \rightarrow L} \). Kirkaldy et al. (1978) give

\[ \Delta^\circ G_{Mn}^{\gamma \rightarrow \delta} = 2.72 \times 10^3 \text{J/mol} - 1.28T \] J/mol

and

\[ \Delta^\circ G_{Mn}^{\gamma \rightarrow L} = 1.20 \times 10^4 \text{J/mol} - 8.50T \] J/mol (4.22)

These two functions are then combined to give

\[ \Delta^\circ G_{Mn}^{\gamma \rightarrow L} = \Delta^\circ G_{Mn}^{\delta \rightarrow \gamma} + \Delta^\circ G_{Mn}^{\gamma \rightarrow L} = 9.25 \times 10^3 - 7.22T \] J/mol (4.23)

A listout of the peritectic program is given in Appendix 3. As with the Ae3 program, a temperature loop was included in the program to increase the accuracy of the final result.

In order to assess the overall accuracy of the program, experimental data were taken from Jernkontoret (1977), in which values for the liquida, solida, and solidification ranges of a wide range of steels have been measured by differential thermal
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Table 4.1: Compositions in wt% of the low-alloy multicomponent steels analysed. Data are taken from Jernkontoret (1977) [Steels 201 → 216], and Howe (1988) [Steels 1 → 26].
<table>
<thead>
<tr>
<th>No.</th>
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<th>Measured Liquidus Temperature/ °C</th>
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Table 4.2: Measured and predicted values for the liquidus temperatures of 22 low-alloy steels.
Figure 4.7: Predicted and measured liquidus temperatures for twenty-two low-alloy steels for primary ferrite and primary austenite solidification. The data are taken from Jernkontoret (1977), and Howe (1988).
analysis at a variety of cooling rates. In addition, newly published experimental data due to Howe (1988), giving the liquidus temperatures of a wide range of steels, were used. The compositions of the steels for which \( \sum_{i=2}^{n} X \leq 6 \) wt% are given in Table 4.1. For this analysis, data from Jernkontoret obtained at the slowest cooling rates (0.1°C/s) were used, since these are expected to be closest to equilibrium. Experimental and calculated values for the liquidus temperatures of the steels given in Table 4.1, are listed in Table 4.2 and plotted in Figure 4.7. It can be seen that agreement is excellent, and actually better than that achieved for the \( \Delta e_3 \), the slight overestimation for the liquidus being conceivably attributable to the measurements being made under continuous cooling conditions.

4.5.2 Solidification as Primary Austenite

The small differences in Gibbs free energy between various equilibria in the Fe-C system means that metastable equilibria should also be considered, since metastable phases may be kinetically favoured. Depending upon the composition and cooling conditions, steels may solidify directly as austenite or ferrite, and, in general, the close proximity of the liquidus surfaces of these two phases means that metastable formation of one phase may occur when equilibrium data indicate that the other phase is the stable one (Fredriksson and Hellner, 1974; Fredriksson, 1976). One particular advantage of using thermochemical calculations is that the \( \gamma / \gamma + L \) phase boundary is readily calculable. High cooling rates can obviate nucleation of the \( \delta \) phase above the peritectic temperature, so that solidification then proceeds according to the austenite-cementite system. Since solute elements have different solubilities and diffusion rates in ferrite and in austenite, segregation is directly influenced by the form of the primary precipitation. Specifically, the diffusion rate of substitutional elements in ferrite is two orders of magnitude greater than in austenite, and consequently segregation during a ferritic solidification process is much smaller than during an austenitic one (Edvardsson et al., 1976). This behaviour has profound significance in welding since solidification as austenite will not only result in differences in solute segregation, but also in the distribution of the inclusions in the weld with respect to the phases that subsequently form.

Figure 4.8 shows the austenite-graphite and austenite-cementite phase diagram, where the stable boundaries are indicated by full lines, those of the austenite-cementite equilibria by dashed lines. This metastable system has been constructed in the program by extrapolating the austenite solidus and austenite liquidus. It
Figure 4.8: Fe-C equilibria of austenite with graphite and cementite. (After O. Kubaschewski, "Iron-Binary Phase Diagrams" (1982), Springer-Verlag, Berlin, FDR, 23-25).
can be seen that the melting point of $\gamma$-Fe is only some 10K lower than the melting point of $\delta$-Fe.

4.5.3 Prediction of Solidification Ranges

Solidification of an alloy with a finite freezing range can allow the formation of an inhomogeneous solid, and the amount of eventual segregation may be directly related to the solidification range of the alloy. It was, therefore, crucial to check the accuracy of the program at predicting the solidus temperatures and solidification ranges of the steels analysed. For steels 201 and 202, which respectively contain 0.11 and 0.12 wt% C, and which solidify through the peritectic as $\delta$-ferrite, the $\delta$ solidus was estimated, to a first approximation, by extrapolation of the $\delta$ solidus line. For the other steels, it was calculated from the austenite solidus. Table 4.3 lists measured and predicted values of the solidus temperatures and solidification ranges for the Jernkontoret steels. These data are plotted in Figures 4.9 and 4.10 respectively. As with the liquidus, it can be seen that the thermodynamic algorithm is an excellent predictor of both the solidus temperature and the solidification range of the steels.

<table>
<thead>
<tr>
<th>No.</th>
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</tr>
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Table 4.3: Calculated and measured solidus and solidification ranges for the steels analysed.
Figure 4.9: Experimental and calculated values for the solidus temperature of a range of twelve low-alloy multicomponent steels. The data are due to Jernkontoret (1977). (0.17wt% carbon corresponds to the peritectic point on the binary Fe-C equilibrium phase diagram, and thus indicates a change in solidification mode for the alloys).
Figure 4.10: Experimental and calculated values for the solidification range of twelve low-alloy steels given in Table 4.1.
Figures 4.11a and b show the entire peritectic region drawn using the computer model. The diagrams show two constant sections through the Fe-C-Mn and Fe-C-Cr phase diagram for 0 and 1.0 wt% manganese, and 0 and 2.0 wt% chromium. Although, the exact composition of the phases in microscopic equilibrium cannot be predicted from a pseudo-binary diagram, trends in compositional change can. Depression of the peritectic and Ae3 temperatures can be seen. Note also stabilization of the austenite phase field and a concomitant contraction of the δ phase field for manganese, and the corresponding expansion of the δ field and contraction of the austenite field when chromium is present.

4.6 CALCULATION OF PARTITION COEFFICIENTS

The partition coefficient of a solute element is a characteristic value showing the degree of microsegregation of an element in an alloy system. To determine the equilibrium partition coefficients of solute elements for multicomponent systems entails time-consuming experiments. Therefore, the application of thermodynamic calculations to the determination of partition coefficients is a logical step, particularly since, for a dilute solution containing small amounts of alloying elements, the contribution from the interaction among the elements to the partition coefficient between δ-ferrite or austenite and liquid iron is negligible (Kagawa et al., 1985). Since the cooling rates encountered in welding are quite high, it can be assumed that segregation arising during solidification is not influenced by subsequent diffusion during cooling from the liquidus (Gretof et al., 1986). By considering the steel at a temperature at which both the ferrite and austenite are in equilibrium, the proportions of these two phases, and their composition (i.e. the partition of the alloy elements) can also be calculated. The partition coefficient of a given solute element is determined using the relationship given in Eqn. 4.11. For example, for the γ/L transformation,

$$X_i = X_i^L A_i$$

(4.24)

where

$$A_i = \frac{\exp \left( \frac{\Delta S_i G^i}{RT} + \epsilon_i L X_i^L \right)}{1 + \epsilon_i^\gamma X_i^L \exp \frac{\Delta S_i G^i}{RT}}$$
Figures 4.11a and b: Fe-C-Mn and Fe-C-Cr phase diagrams. The diagrams were constructed using points generated by the computer model. (Note: for simplicity, the three-phase peritectic region has been kept as a straight line).
Figures 4.12a and b: Calculated and experimental values for the equilibrium partition coefficients of solute elements for a) δ-ferrite and liquid iron, and b) austenite and liquid iron. Lines are lines of ideality.
4.7 SUMMARY

Standard free energy changes and activity data for iron and its binary and ternary alloys have been used to evaluate the general linear series (Wagner) expansion of the activity coefficient, and these have themselves been used to generate an accurate thermodynamic determination of equilibrium multicomponent Fe-C-X transformation temperatures. A computer program has been written which accurately describes the influence of low concentrations of alloying elements on the $\Delta_{E3}$ equilibrium temperature of low-alloy steels containing for up to 1.8 wt% C. Using the method due to Baganis and Kirkaldy (1978), the phase boundary is calculated using empirical data to estimate the Gibbs free energy of the participating phases in the multicomponent system, and the resultant deviation of the phase boundary from that of the binary Fe-C system is then found. New elements (V, Nb, W, Co) have been incorporated to the program, and revised values for $\Delta^0G_o$, $\Delta^0H_o$, and $T_o$ have been used. In addition, discrepancies with the Fe-Mn, Fe-Ni, and Fe-Nb systems have been resolved. The program has been shown to be valid for significant additions of Mn, Si, Ni, Cr, Mo, Cu, V, Nb, W and Co.

The peritectic region of the phase diagram has been calculated, with each phase boundary being treated individually, and for the first time its accuracy evaluated. Results obtained by calculation have been compared with experimental data for the liquida and solida of a range of low-alloy multicomponent steels, and found to be in extremely good agreement. A good ability to predict the solidification range, which strongly influences the amount of solute segregation, was also obtained. Finally, an attempt has been made to estimate the amount of partitioning for alloying elements between $\delta$- and liquid iron, and between austenite and liquid iron, and agreement with observed results was fair. This model has been shown to accurately predict the modifications to the Fe-Fe$_3$C phase diagram of any given set of alloying elements, in the following range: C $\leq$ 1.8wt%, Mn $< 3.0\%$, Ni $< 2.5\%$, Cr $< 2.5\%$, Co $< 2\%$, Mo $< 1.5\%$, rest (including Si) $\leq 1.0\%$. This covers the largest proportion of steels used in welding fabrication.

The practical limitations of the program arise from two sources, namely, the limitations of the theory itself, in particular the inability to account for solute-solute interactions, since it is only strictly correct for infinitely dilute solutions, and inadequate experimental data for the pure binary systems with iron as one component. It is anticipated that these source data will be refined as development
of the program continues.
REFERENCES

COHEN, M. (1962), Trans. AIME, 224, 638-656.


SCHURMANN, E., VON SCHWEINICHEN, J., VOLKER, R., and FISCHER, H.


CHAPTER 5

A MODEL FOR THE STRENGTH OF THE AS-DEPOSITED REGIONS OF LOW-ALLOY STEEL WELD METALS

5.1 NOMENCLATURE

The following nomenclature is used in this Chapter:

\( \alpha \) allotropic ferrite
\( \alpha_a \) acicular ferrite
\( \alpha_w \) Widmanstätten ferrite
\( \delta \) delta-ferrite
\( \Delta \sigma \) increment in yield stress
\( \gamma \) austenite
\( \varepsilon \) true strain
\( \bar{\varepsilon} \) true average strain
\( \varepsilon^I_p \) true plastic strain in softer phase of a dual-phase steel
\( \varepsilon^II_p \) true plastic strain in harder phase of a dual-phase steel
\( \varepsilon_{UTS} \) true strain at ultimate tensile stress
\( \varepsilon_y \) true strain at yielding
\( \dot{\varepsilon} \) strain rate
\( \mu \) shear modulus of iron-base solid-solution single crystal
\( \tau_y \) shear stress of iron-base solid-solution single crystal
\( \sigma \) true stress
\( \sigma_a \) microstructural strengthening due to allotropic ferrite
\( \sigma_a \) microstructural strengthening due to acicular ferrite
\( \sigma_{Fe} \) yield strength of fully annealed pure iron as a function of temperature
and strain rate

\( \sigma_{\text{micro}} \) strengthening due to microstructure

\( \sigma_{\text{micro}_y} \) strengthening due to microstructure at the yield stress

\( \sigma_{\text{micro}_{UTS}} \) strengthening due to microstructure at the ultimate tensile stress

\( \sigma_{SS_i} \) solid solution strengthening imparted due to an alloying element \( i \)

\( \sigma_{UTS} \) ultimate tensile stress

\( \sigma_w \) microstructural strengthening due to Widmanstätten ferrite

\( \sigma_y \) yield stress

\( \Omega \) regression function defined in Eqn. 5.19

\( A \) area of cross-section of a tensile specimen

\( a, b \) regression coefficients used in the analysis of strength

\( C \) regression constant used in the analysis of strength

\( C_{\text{equiv}} \) carbon equivalent

\( i \) weld metal alloying element (\( i = 1, \ldots, k \))

\( j \) number of weld analysed (\( j = 1, \ldots, 35 \))

\( K \) strength coefficient

\( K_{\alpha} \) microstructural strength coefficient for allotriomorphic ferrite

\( K_a \) microstructural strength coefficient for acicular ferrite

\( K_w \) microstructural strength coefficient for Widmanstätten ferrite

\( n \) strain hardening exponent

\( n_{\alpha} \) microstructural strain-hardening exponent for allotriomorphic ferrite

\( n_a \) microstructural strain-hardening exponent for acicular ferrite

\( n_w \) microstructural strain-hardening exponent for Widmanstätten ferrite

\( P \) applied load

\( T \) absolute temperature

\( V_{\alpha} \) volume fraction of allotriomorphic ferrite in weld microstructure
5.2 INTRODUCTION

Much fundamental work has recently been done on the prediction of the microstructure of steel weld deposits (Bhadeshia et al., 1985; Bhadeshia et al., 1986; Svensson et al., 1986), and it is now possible to estimate the as-welded microstructure as a function of chemical composition and thermal history. While the work on microstructure prediction has made good progress, it is the properties of welds which ultimately determine the quality of that weld. The aim of this work is to try and predict strength as a function of alloy concentration and microstructure, and also over a wide temperature range. Many welds are used or tested at non-ambient temperatures, and it is then not sufficient only to be able to predict their strength at room temperature.

The solidification of low-alloy steel weld deposits starts with the epitaxial growth of delta-ferrite (δ) from the parent plate grains at the fusion boundary. The high temperature gradients involved in arc welding cause solidification to proceed in a cellular manner with the grains having their major axes following the direction of maximum heat flow. On further cooling, allotriomorphs of austenite (γ) nucleate at the δ/δ cell boundaries, and anisotropic γ growth along these boundaries leads to the formation of columnar austenite grains which closely resemble the original δ-ferrite morphology. On cooling to temperatures below the Ae₃ temperature, the first phase to form is allotriomorphic ferrite (α). The fer-
rite nucleates at the columnar austenite grain boundaries, which rapidly become covered with a nearly uniform layer of α. Following this, Widmanstätten ferrite (αw) nucleates at the α/γ boundaries and grows by a displacive mechanism in the form of thin, wedge-shaped plates at a rate approximately controlled by the diffusion of carbon in the austenite ahead of the interface. At the same time, a third phase, acicular ferrite (αa), which consists of a series of non-parallel arrays of bainite laths, nucleates intragranularly (Yang and Bhadeshia, 1986; Bhadeshia, 1987). Finally, very small volume fractions of “microphases” are found within the acicular ferrite consisting of mixtures of martensite, degenerate pearlite and retained austenite, all resulting from the austenite remaining untransformed after α, αw, and αa have formed. However, microphases comprise typically only 1–3% of the weld microstructure, and it is the three morphologically distinct phases—allotriomorphic, Widmanstätten, and acicular ferrite— which can be said to form the primary microstructure (Bhadeshia et al., 1985).

5.3 METHOD

It is normal practice to express the weld metal strength as a function of the alloying elements present. Equations used in such analyses typically state the yield stress as follows:

\[
\sigma_y = C + a \text{ wt\% Mn} + b \text{ wt\% Si} + \ldots
\]  

(5.1)

where \( C \) is a constant,

and \( a, b, \ldots \) are supposed to define the role of alloying additions (Bailey and Pargeter, 1978; Bosward and John, 1979; Evans, 1981).

Identical equations have been derived to allow for the estimation of the microstructure of the ultimate tensile strength of a weld, \( \sigma_{UTS} \) (Bailey and Pargeter, 1978; Samuel, 1984). \( C \) and the other coefficients are found by regression analysis on a given set of data, and, as such, are highly specific to that set of data, and doubtful in extrapolation. This approach is inadequate, as shown by a wide spread of coefficients obtained by different workers for the strengthening effects of individual elements, (summarised by Judson (1982), and Abson and Pargeter (1986)). (The diversity is hardly surprising, since the weld strength is a function
of the heat input, interpass temperature, columnar grain size, dislocation density, &c.). More importantly, such an equation ignores the effects of thermal history since the microstructural reheating that occurs during multi-pass welding, and also post-weld heat treatment, does not change the composition of a weld, and yet alters its strength. The strength clearly must also be a function of the microstructure. Most welding variables (e.g. heat input, preheat temperature, welding geometry), manifest themselves in altering the microstructure. Also, it does not allow for any means by which the strength of a weld at yield and at UTS may be related.

In a multi-phase system, such as a weld deposit, the overall strength will be strongly related to the strengths and volume fractions of the phases present, an optimum high strength, high toughness, microstructure being associated with a high proportion of acicular ferrite. The simplest assumption from this would be that the mean strength of the weld should be linearly related to the strengths and abundances of the phases present (see, for example, Tweed and Knott, 1987a). This "rule of mixtures" is most commonly used for predicting the strength of composite materials, when a ductile matrix is reinforced by brittle (Kelly, 1966), or even ductile (Ahmad and Barranco, 1970; Davis and Scala, 1973), continuous fibres, although strictly the rule shows the upper bound of the strength since the fibres and the matrix are assumed to fail simultaneously (Fukuda et al., 1981).

The following model is based on the assumption that the strength can be factorised into components due to the intrinsic strength of iron, solid solution strengthening, and the contributions from the three major phases (α, αw, αa) which constitute the microstructure:

\[
\sigma = \sigma_{Fe} + \sum_{i=1}^{k} \sigma_{SS_i} + \sigma_{micro} \tag{5.2}
\]

where \(\sigma_{Fe}\) is the strength of fully annealed pure iron as a function of temperature and strain rate,

\(\sigma_{SS_i}\) is the solid solution strengthening due to an alloying element \(i\), †

† Allotriomorphic ferrite appears in weld deposits to grow without the redis-
and \( \sigma_{\text{micro}} \) is the strengthening due to microstructure.

Substituting for \( \sigma_{\text{micro}} \), Eqn. 5.2 may be written,

\[
\sigma = \sigma_{\text{Fe}} + \sum_{i=1}^{k} \sigma_{\text{SS},i} + V_{\alpha} \sigma_{\alpha} + V_{\omega} \sigma_{\omega} + V_{\alpha} \sigma_{\alpha}
\]  

(5.3)

where \( V_{\alpha}, V_{\omega}, \) and \( V_{\omega} \) are the volume fractions of the allotriomorphic, acicular, and Widmanstätten ferrite phases respectively.

To express the stress as a function of strain, it is assumed that the true stress/true strain curve in the plastic region can be approximated by (Nadai, 1931)

\[
\sigma = K \epsilon^n
\]

(5.4)

where \( \epsilon \) is the true strain

\( n \) is the strain hardening exponent

and \( K \) is the strength coefficient, equal to the value of the flow stress at \( \epsilon^n = 1.0 \).

This equation describes a state of stable plastic deformation, and, although alternative descriptions exist, it is this equation which has been most successfully applied by various workers to describing weld metal tensile behaviour in this regime (Tweed, 1987b; McRobie and Knott, 1985).

Using this relationship, Eqn. 5.3 has been further extended to become

\[
\text{tribution of substitutional alloying elements during transformation (Bhadeshia et al., 1985), } \alpha_w \text{ grows by a paraequilibrium mechanism (Bhadeshia, 1987), and } \alpha_a \text{ growth is diffusionless (Yang and Bhadeshia, 1986; Strangwood and Bhadeshia, 1986) with subsequent rejection of carbon into the residual austenite. This means that the solid solution strengthening contribution from substitutional elements is identical for all three phases.}
\]
where $K_\alpha$, $K_w$, and $K_a$ are strength coefficients, and $n_\alpha$, $n_w$, and $n_a$ are strain-hardening exponents for allotriomorphic ferrite, Widmanstätten ferrite, and acicular ferrite respectively.

Since the layers of allotriomorphic ferrite that grow at the $\gamma$ grain boundaries do not usually extend very far into the grains of austenite, the assumption is made that the allotriomorphic ferrite grain size, as limited by hard impingement along the $\gamma$ grain boundaries, does not vary significantly between welds in low-alloy steels. The plate morphologies of $\alpha_w$ and $\alpha_a$ are generated by displacive transformation, and it is also assumed that any variations in their sizes are not significant, relevant to the other variables (Bhadeshia and Svensson, 1988). The austenite grain size is ignored in this calculation because the grains are usually too large to contribute significantly to strength.

In order to calculate the strength of pure iron, $\sigma_{Fe}$, and the effect of alloying elements on solid solution strengthening, $\sigma_{SS}$, published data have been collected for the temperature range 100–750K. Data for the normal yield stress of pure annealed polycrystalline b.c.c. iron as a function of strain rate and temperature have been taken from three sources (Conrad and Fredrick, 1962; Altshuler and Christian, 1967; Kimura et al., 1981). The individual effects of five ferrous alloying elements (Mn, Si, Ni, Cr, and Co) on the yield strength of pure iron as a function of concentration and temperature are obtained from work due to Leslie (1972), and information on the effect of nitrogen on the strength of high purity iron, as a function of temperature (at a strain rate similar to that used by Leslie), is obtained from the work of Kitajima et al. (1979). The detailed data were represented on computer as cubic splines which allow a continuous representation of $\sigma_{SS}$ with temperature (Hayes, 1974). Thus although in this work only room temperature strength is considered, in fact, $\sigma_{SS}$ can now be estimated from 100 to 750K. Nitrogen is assumed to be in solid solution, and strain ageing effects in the as-welded microstructure are taken as negligible. It should be noted that many elements, such as nickel, manganese, and nitrogen, give softening at certain concentrations and
temperatures. This occurs because distortion of the atomic lattice, particularly at low temperatures, can locally reduce the Peierls-Nabarro barrier and facilitate slip.

The solid solution strengthening of iron at 298K has been determined for phosphorus (Leslie, 1972), molybdenum, aluminium, and vanadium (Takeuchi, 1969), titanium (Takeuchi et al., 1968), and boron (Irvine and Pickering, 1963), and, in the absence of further data, the strengthening due to these elements is taken to be athermal. Although this is a simplification, it is not a serious one since it has become apparent from this work that typically not less than 90% of the solid solution strengthening in a low-alloy steel weld deposit is due to manganese, silicon, and nitrogen. Where necessary, shear yield stress data were converted into normal yield stress data using the Tresca criterion (Dieter, 1976).

The effect of carbon on the strength of ferrite has been investigated by Chilton and Kelly (1968), and Norström (1976). However, the solubility of carbon in ferrite in contact with cementite decreases with temperature, and at room temperature is less than 10^{-3}at\% (Hansen, 1958), and consequently the solid solution strengthening due to carbon need only be included for temperatures greater than 200°C. In fact, during the cooling of a weld, the ferrite grows in contact with austenite rather than cementite, so that it is the solubility with respect to cementite that needs to be considered, but this is not expected to be very different (Bhadeshia, 1982). Oxygen and sulphur are assumed to be present in the form of inclusions, and not to be in solid solution (Steel, 1972).

Although data for a variety of strain rates had been collated, (typically in the range 5.0x10^{-6} to 10^{-2}s^{-1}), for the following work a value of 2.5x10^{-4}s^{-1}, as used by Leslie, was chosen. A listout of the program written to allow the calculation of \(\sigma_{Fe} \) and \(\sum_{i=1}^{k} \sigma_{SS} \), as a function of temperature is given in Appendix 3.

In order to calculate \(\sigma_{a}, \sigma_{w}, \) and \(\sigma_{w}, \) data on 35 welds was taken from four sources [Widgery (1976), Bailey and Pargeter (1978), Cunha et al. (1982), and Dowling et al., (1986)] for which experimental results for yield stress and ultimate tensile stress from primary (unrefined) all-weld metal specimens were given, together with the volume fractions of \(\alpha, \alpha_{w}, \) and \(\alpha_{a} \) comprising them. The welding conditions are all different, but these differences are all taken into account, since

\[\uparrow \text{Popular earlier data from Lacy and Gensamer (1944) were not used since the interstitial content of their alloys was not rigorously controlled.}\]
Figure 5.1: Effect of solutes on the strength of polycrystalline iron as a function of temperature for 3 at.% concentration of solutes.

\[ \Delta \sigma = \text{increment in yield stress.} \ (\dot{\epsilon} = 2.5 \times 10^{-4} / \text{s}). \]

Figure 5.2: Strength of iron-base solid solution single crystals; the ratio of the resolved shear stress at the lower yield point to shear modulus as a function of atomic concentration of solute. (After Takeuchi, S. (1969), *J. Phys. Soc. Japan*, 27, 167).
they cause different resulting microstructures.

From Eqn. 5.2, the strengthening due to microstructure at the yield stress

\[
\sigma_{\text{micro}_y} = \sigma_y - \sigma_{\text{Fe}} - \sum_{i=1}^{k} \sigma_{SS_i}
\]  

(5.6a)

where \( \sigma_y \) is the yield stress.

Similarly

\[
\sigma_{\text{micro}_\text{UTS}} = \sigma_{\text{UTS}} - \sigma_{\text{Fe}} - \sum_{i=1}^{k} \sigma_{SS_i}
\]  

(5.6b)

where \( \sigma_{\text{UTS}} \) is the ultimate tensile stress.

At the yield stress

\[
\sigma_{\text{micro}_y} = V_a K_\alpha (\epsilon_y)^{n_\alpha} + V_w K_w (\epsilon_y)^{n_w} + V_a K_\alpha (\epsilon_y)^{n_\alpha}
\]  

(5.7)

where \( \epsilon_y \) is the true strain at yielding.

Since proof stress is usually measured at 0.2% plastic strain, a fair assumption for \( \epsilon_y \) is to take it as corresponding to the point of 0.2% plastic strain. Accordingly, \( \epsilon_y \) was taken as 0.002.

The ultimate tensile strength should now be considered. The onset of necking corresponds to the transition from smooth necking to local fracture and may be defined by the Considère construction (Considère, 1885).

The true stress
\[ \sigma = \frac{P}{A} \]  \hspace{1cm} (5.8)

where \( P \) is the applied load

and \( A \) is the area of cross-section of the tensile specimen.

Necking occurs when an increase in strain produces no increase in load, i.e. 
\[ dP = 0 \]

Therefore, from Eqn. 5.8

\[ dP = A \, d\sigma + \sigma \, dA = 0 \]  \hspace{1cm} (5.9)

Therefore

\[ \frac{d\sigma}{\sigma} = -\frac{dA}{A} \]  \hspace{1cm} (5.10)

During deformation, the volume of the specimen is taken as constant, i.e.

\[ d(Al) = A \, dl + l \, dA = 0 \]  \hspace{1cm} (5.11)

Therefore

\[ \frac{dl}{l} = -\frac{dA}{A} \equiv d\varepsilon \]  \hspace{1cm} (5.12)

Combining Eqns. 5.10 and 5.12 gives

\[ \frac{d\sigma}{d\varepsilon} = \sigma \]  \hspace{1cm} (5.13)

For \( \sigma = K\varepsilon^n \), therefore, Eqn. 5.13 means

\[ \frac{d\sigma}{d\varepsilon} = nK\varepsilon^{n-1} = K\varepsilon^n \]  \hspace{1cm} (5.14)
Therefore

\[ \varepsilon = n \] \hspace{1cm} (5.15)

Therefore, necking occurs when the true strain equals the strain-hardening exponent. Thus, the strengthening due to microstructure at the ultimate tensile strength, \( \sigma_{\text{microUTS}} \), may be written

\[
\sigma_{\text{microUTS}} = V_a K_a (n_a)^{n_a} + V_w K_w (n_w)^{n_w} + V_a K_a (n_a)^{n_a}
\] \hspace{1cm} (5.16)

It should be emphasized that the coefficients \( K_a, K_w, \) and \( K_a, \) and \( n_a, n_w, \) and \( n_a \) are not directly comparable to the coefficients \( K \) and \( n \) in Eqn. 5.4, since the strengthening due to pure annealed iron, and that due to microstructure has been removed. The different values of strain in the three phases takes into account that the post-yield strain will not be uniformly distributed, with the harder constituents deforming less (Tomota et al., 1976; Tweed and Knott, 1987b). Realistically, the phases have different yield strengths and deformation should be inhomogeneous. However, in the absence of detailed data on the deformation characteristics of the individual phases, and on the grounds that the phases are not too dissimilar, we assume that the strain in any phase is the same as the average overall sample strain, i.e. deformation is homogeneous. For example, Figure 5.3 shows the case calculated for a ferrite/martensite dual-phase steel, when the mechanical properties of the constituent phases are quite different. It can be seen that although the initial strain increments (as a function of the average strain, \( \bar{\varepsilon} \)) are quite different in the two phases, as the softer phase work-hardens, the rate of straining in the two phases becomes about equal. Since the true strain at the ultimate tensile stress is very much greater than the true strain at yielding, it is a good approximation to assume homogeneous deformation at the ultimate tensile stress, although near the yield point it is very likely that the softest of the phases will yield first.

The data used give experimentally determined values \( \sigma_{\text{micro}}, \sigma_{\text{microUTS}}, V_a, V_w, \) and \( V_a \). For a given weld, let

\[
X = \sigma_{\text{micro}} - V_a K_a (0.002)^{n_a} - V_w K_w (0.002)^{n_w} - V_a K_a (0.002)^{n_a}
\] \hspace{1cm} (5.17)
Figure 5.3: Calculated cumulative plastic strain in hard phase, $\varepsilon_p^{II}$, versus that in the soft phase, $\varepsilon_p^I$ for ferrite/martensite dual-phase steel. (After H. K. D. H. Bhadeshia and D. V. Edmonds, *Met. Sci.*, 14, (2), 41-49).
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Table 5.1: Calculation of $\sigma_{micro_y}$ and $\sigma_{micro_{UTS}}$ for welds used in the analysis of strain hardening coefficients.
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<td>0.53</td>
</tr>
<tr>
<td>37</td>
<td>149</td>
<td>279</td>
<td>0.37</td>
<td>0.25</td>
<td>0.38</td>
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<td>0.29</td>
<td>0.24</td>
<td>0.47</td>
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<td>41</td>
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<td>0.41</td>
<td>0.16</td>
<td>0.43</td>
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<tr>
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<td>295</td>
<td>0.46</td>
<td>0.08</td>
<td>0.46</td>
</tr>
<tr>
<td>13</td>
<td>124</td>
<td>207</td>
<td>0.35</td>
<td>0.24</td>
<td>0.41</td>
</tr>
<tr>
<td>14</td>
<td>322</td>
<td>417</td>
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<td>0.92</td>
<td>0.0</td>
</tr>
<tr>
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<td>216</td>
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<td>0.18</td>
<td>0.03</td>
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</tr>
<tr>
<td>16</td>
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<td>0.25</td>
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<tr>
<td>17</td>
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<td>333</td>
<td>0.24</td>
<td>0.07</td>
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<td>18</td>
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<td>19</td>
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<td>323</td>
<td>0.36</td>
<td>0.44</td>
<td>0.20</td>
</tr>
<tr>
<td>B1</td>
<td>365</td>
<td>398</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>B4</td>
<td>356</td>
<td>406</td>
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<td>1.0</td>
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<tr>
<td>K8</td>
<td>309</td>
<td>409</td>
<td>0.05</td>
<td>0.03</td>
<td>0.92</td>
</tr>
</tbody>
</table>

Table 5.2: Summary of $\sigma_{micro_y}$ and $\sigma_{microUTS}$ together with volume fractions of phases present in the welds.
and let

\[ Y = \sigma_{\text{microU}} - V_\alpha K_\alpha (n_\alpha)^{n_\alpha} - V_w K_w (n_w)^{n_w} - V_a K_a (n_a)^{n_a} \]  \hspace{1cm} (5.18)

Eqn. 5.16 defines the condition that all phases achieve plastic instability at the same strain at which the sample as a whole begins to neck. The values of \( K_\alpha, n_\alpha, \ldots \) thus obtained will reflect the different hardening rates necessary in order to satisfy this condition, so that it is expected that the allotriomorphic ferrite, which starts off relatively weak should have a high value of strain-hardening exponent, \( n_\alpha \).

By the least squares method, and giving the values for \( \sigma_{\text{microU}} \) and \( \sigma_{\text{microU}} \) equal weightings, the best fit for the data is when the function \( \Omega \) is a minimum, where

\[ \Omega\{K_\alpha, K_w, K_a, n_\alpha, n_w, n_a\} = \sum_{j=1}^{35} X^2 + \sum_{j=1}^{35} Y^2 \]  \hspace{1cm} (5.19)

where \( j \) is the number of sets of data analysed \((j = 1, \ldots, 35)\).

This minimum can be found by taking the partial derivatives of Eqn. 5.14 with respect to \( K_\alpha, K_w, K_a, n_\alpha, n_w \), and \( n_a \) as follows:

\[ \frac{\partial \Omega}{\partial K_\alpha} = 2 \sum_{j=1}^{35} \{ X.V_{\alpha_i} (0.002)^{n_\alpha} \} + 2 \sum_{j=1}^{35} \{ Y.V_{\alpha_i} (n_\alpha)^{n_\alpha} \} \]  \hspace{1cm} (5.20a)

\[ \frac{\partial \Omega}{\partial K_w} = 2 \sum_{j=1}^{35} \{ X.V_{w_i} (0.002)^{n_w} \} + 2 \sum_{j=1}^{35} \{ Y.V_{w_i} (n_w)^{n_w} \} \]  \hspace{1cm} (5.20b)

\[ \frac{\partial \Omega}{\partial K_a} = 2 \sum_{j=1}^{35} \{ X.V_{a} (0.002)^{n_a} \} + 2 \sum_{j=1}^{35} \{ Y.V_{a_i} (n_a)^{n_a} \} \]  \hspace{1cm} (5.20c)
\[
\frac{\partial \Omega}{\partial n_\alpha} = 2 \sum_{j=1}^{35} \{X.V_\alpha, K_\alpha \ln(0.002) \cdot (0.002)^{n_\alpha}\} \\
+ 2 \sum_{j=1}^{35} \{Y.V_\alpha, K_\alpha (n_\alpha)^{n_\alpha} \cdot (1 + \ln(n_\alpha))\} \\
(5.20d)
\]

\[
\frac{\partial \Omega}{\partial n_w} = 2 \sum_{j=1}^{35} \{X.V_w, K_w \ln(0.002) \cdot (0.002)^{n_w}\} \\
+ 2 \sum_{j=1}^{35} \{Y.V_w, K_w (n_w)^{n_w} \cdot (1 + \ln(n_w))\} \\
(5.20e)
\]

\[
\frac{\partial \Omega}{\partial n_a} = 2 \sum_{j=1}^{35} \{X.V_a, K_a \ln(0.002) \cdot (0.002)^{n_a}\} \\
+ 2 \sum_{j=1}^{35} \{Y.V_a, K_a (n_a)^{n_a} \cdot (1 + \ln(n_a))\} \\
(5.20f)
\]

Eqns. 5.15a-f will all equal zero when a valid solution is obtained. In order to find this condition, a NAG† FORTRAN subroutine was used which estimates partial derivatives of the functions supplied from their arguments, and uses these to rapidly reach the solution nearest to a set of supplied “best guess” values. This achieved using a convergence technique described elsewhere (Powell, 1970).

5.4 CHOICE OF GUESSED VALUES

Since Eqns. 5.15a-f were non-linear, there would be more than one solution for the equations, and so the selection of the initial guess values would be extremely important. Welds Q and 14, which have very high percentages of acicular ferrite and Widmanstätten ferrite respectively (see Table 5.2) were treated as single phase microstructures, and knowing \(\sigma_y, \sigma_{UTS}, \) and \(\sum_{i=1}^{k} \sigma_{SS_i}\), values for \(K_w, n_w, K_a,\) and \(n_a\) were found using Eqn. 5.5. \(K_a\) and \(n_a\) were then found by substituting

† ©National Algorithms Group Ltd., 256 Banbury Road, Oxford, U.K.
these approximate values into Eqn. 5.5 using the data for weld 67, which contains 46% $a$. The values thus derived are as follows:

\[
\begin{align*}
K_\alpha &= 202 \text{ MPa} \\
K_w &= 504 \text{ MPa} \\
K_a &= 526 \text{ MPa}
\end{align*}
\]

\[
\begin{align*}
n_\alpha &= 0.595 \\
n_w &= 0.072 \\
n_a &= 0.094
\end{align*}
\]

### 5.5 RESULTS

After 22 iterations, the arguments of Eqns. 5.20a-f were all less than $10^{-6}$, and the following values for the coefficients were obtained:

\[
\begin{align*}
K_\alpha &= 124 \text{ MPa} \\
K_w &= 478 \text{ MPa} \\
K_a &= 499 \text{ MPa}
\end{align*}
\]

\[
\begin{align*}
n_\alpha &= 0.644 \\
n_w &= 0.0812 \\
n_a &= 0.103
\end{align*}
\]

Substituting in Eqn. 5.5 gives two general equations:

\[
\sigma_{\text{micro}} = 2.26V_\alpha + 289V_w + 263V_a \tag{5.21a}
\]

\[
\sigma_{\text{micro}U\tau S} = 94V_\alpha + 390V_w + 395V_a \tag{5.21b}
\]

More generally, the overall strength of a weld may be written:

\[
\sigma = \sigma_{Fe} + \sum_{i=1}^{k} \sigma_{SS_i} + V_\alpha \cdot 124e^{0.644} + V_w \cdot 478e^{0.0812} + V_a \cdot 499e^{0.103} \tag{5.22}
\]

Measured and calculated values for yield strength and ultimate tensile strength for the 35 welds are plotted in Figures 5.4 and 5.5 respectively.
Figure 5.4: Measured values for yield strength plotted against values predicted using Eqn. 5.21a. (Correlation coefficient = 0.85).
Figure 5.5: Measured and predicted values for ultimate tensile strength. (Correlation coefficient = 0.91).
5.6 USING THE MODEL

Figures 5.4 and 5.5 show that the overall ability of the equations to predict the tensile strength of the as-deposited regions of a wide variety of welds and welding conditions is very good. It can be seen from Eqn. 5.21a that allotriomorphic ferrite has a yield strength only a little greater than that of pure iron, whereas acicular ferrite and Widmanstätten ferrite are much stronger. Widmanstätten ferrite is expected to be stronger than allotriomorphic ferrite. $\alpha_w$ grows by a displacive transformation mechanism, and should have a higher dislocation density (Bhadeshia, 1981). Furthermore, Widmanstätten ferrite laths in weld deposits typically have carbides aligned along them, and these will contribute to the strength. The microphases present in acicular ferrite would contribute to the strength of $\alpha_a$ in a similar way. Although, allotriomorphic ferrite work-hardens much more than Widmanstätten ferrite and acicular ferrite with $n_\alpha \gg n_a > n_w$, its strength at UTS is still much less than that of the other two phases whose microstructural contributions are effectively identical. It should be noted that to predict weld metal yield stress and ultimate tensile stress is of potential use in fatigue analysis, since the ratio between the two will give an indication of susceptibility to fatigue crack propagation (A. S. M., 1985).

Figure 5.6 shows the true stress/true strain curve for a hypothetical Fe-0.06C-0.35Si-1.0Mn wt% weld metal microstructure containing equal volume fractions of allotriomorphic ferrite, Widmanstätten ferrite, and acicular ferrite, calculated using Eqn. 5.22. The figure illustrates how the relative strengthening contributions of the three phases alter during plastic deformation. It can be seen that allotriomorphic ferrite provides little strengthening in the early stages of plastic deformation, but work-hardens rapidly as deformation progresses to contribute appreciably to the overall strength. Note that the relatively large plastic strains have caused the elastic region to be compressed into the $y$ axis. Such results provide an explanation for the recent experimental observations of Oldland (1985), who worked on low-alloy C-Mn and C-Mn-Nb SA weld metals containing up to 60% allotriomorphic ferrite, and noted that weld metal yield strength and ultimate tensile strength correlated strongly with the volume fraction of allotriomorphic ferrite present in the welds. This can be appreciated quantitatively from Eqns. 5.21a and b, where a small change in $V_\alpha$ will lead to a large change in observed strength.

In order to demonstrate the general applicability of the model for strength, the
Figure 5.6: Calculated true stress/true strain curves up to the ultimate tensile stress for a weld metal with a composition Fe-0.06C-0.35Si-1.0Mn wt% comprising one third allotriomorphic ferrite, Widmanstätten ferrite, and acicular ferrite.
tensile behaviour of a series of low-alloy C-Mn welds containing 0.35 wt% Si, with systematically varying carbon and manganese concentrations has been calculated using volume fractions which are themselves calculated using the phase transformations model for the calculation of weld metal microstructure described earlier (Bhadeshia et al., 1985). Precise details of the calculation of the volume fractions of the phases in the welds described are given in Bhadeshia and Svensson (1988). The carbon and manganese contents were chosen, together with the fixed percentage of silicon, to reflect simple nominal chemical compositions that might be typical of low-alloy steel weld deposits, although, in fact, the model is able to accommodate all of the major elements that are commonly found in low C-Mn weld metals. Figures 5.7a and b show how the yield stress and ultimate tensile stress vary with manganese content for different carbon concentrations. The results are extremely interesting. First of all, it can be seen that additions of both manganese and carbon will lead to an increase in weld metal tensile strength. Manganese provides solid solution strengthening, and both manganese and carbon act to increase the size of the austenite phase field, and so reduce the driving force for ferrite formation at any given temperature. This behaviour promotes the formation of acicular ferrite, at the expense of allotriomorphic ferrite, and also Widmanstätten ferrite. It can also be seen how the change from 0.03 wt% C to 0.06 wt% C leads to a much greater increase in tensile strength than when going from 0.06 wt% C to 0.10 wt% C. This explanation for this is that as the carbon concentration decreases to low levels, the kinetics of the allotriomorphic ferrite transformation increase rapidly. The concentration profile of the carbon ahead of the advancing interface is strongly dependent upon $\bar{x}$, the average carbon concentration in the alloy, and becomes very steep (i.e. diffusion away from the interface becomes very rapid) as the carbon concentration tends to zero. Thus, increasing the carbon content from 0.03 wt% C 0.06 wt% C has a much greater effect upon the ultimate volume fraction of allotriomorphic ferrite, and so mechanical properties, than increments at higher carbon concentrations.

This observation provides an answer as to why two empirical different carbon equivalent equations have emerged over the years. The carbon equivalent of a steel is a measure of its weldability, and is most usually calculated as follows (Easterling, 1983):

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Figures 5.7a and b: Calculation of (a) yield stress, and (b) ultimate tensile stress for a series of hypothetical welds deposited in the flat position. (Nominal heat input = 1 kJ/mm). The welds contain 0.35wt% Si, and varying concentrations of carbon and manganese.
This equation describes approximately how the alloying elements present will alter the transformation behaviour of the steel during welding, and it is generally supposed that a steel will be weldable if \( C_{\text{equiv}} < 0.4 \). At low carbon concentrations, however, Eqn. 5.22 is found to be unreliable, and an empirical equation due to Ito and Bessayo (1968) is preferred:

\[
C_{\text{equiv}} = C + \frac{\text{Mn}}{6} + \frac{\text{Cr} + \text{Mo} + \text{V}}{5} + \frac{\text{Cu} + \text{Ni}}{15} + 6 + 5 + 15 \quad (5.23)
\]

It can be immediately seen that the apparent influence of substitutional alloying elements on weldability is been found to be much less for low-carbon steels as indicated by the larger denominators in Eqn. 5.23. This can be understood in terms of the greatly increased potency of carbon additions at low carbon concentrations, when the influence of substitutional alloying elements on weldability relative to that of carbon is correspondingly reduced. At higher carbon concentrations, they have a more noticeable effect.

Figures 5.8a and b plot the true stress/true strain curve for a set of welds with varying manganese and carbon concentrations. The strain experienced during uniform deformation is readily calculable from \( \sigma_y \) up to the ultimate tensile stress. The ultimate tensile stress is calculated from the criterion specified in Eqn. 5.18. It can be seen that ductility, as indicated by true strain, increases with decreasing tensile strength.

Finally, it should be said that an important conclusion of this work is that, in terms of mechanical properties, there is no advantage in increasing the amount of Widmanstätten ferrite in a weld deposit. Acicular ferrite has superior mechanical properties to those of Widmanstätten ferrite (Otterberg et al., 1980; Dolby, 1982; Abson and Pargeter, 1986), and yet, as this work shows, has equivalent tensile properties.

5.7 SUMMARY

The strength of the primary regions of a range of low-alloy steel weld metals has
Figures 5.8a and b: True stress/true strain curves for six hypothetical welds calculated up to the ultimate tensile stress for varying (a) carbon and (b) manganese concentrations. The deposit base compositions are (a) 1.0 wt% Mn-0.35 wt% Si, and (b) 0.06 wt% C-0.35 wt% Si. (Welding conditions are as in Figure 5.7).
been investigated as a function of microstructure and composition. It is demonstrated that the yield strength and ultimate tensile strength may be estimated by summing the strength of pure iron, the solid solution strengthening due to the alloying elements, and a contribution due to microstructure. The microstructural contribution is further factorised into the individual effects of the three phases: allotriomorphic ferrite \((\alpha)\), Widmanstätten ferrite \((\alpha_w)\), and acicular ferrite \((\alpha_a)\). It has been possible to rationalise data from a wide range of welds using a unique set of parameters for the model which describing the flow stress and work-hardening behaviour of the individual phases.

The model has been used to construct true stress/true strain curves for a series of hypothetical welds with a representative range of chemical compositions. Calculated tensile behaviour has been interpreted in terms of the kinetics of microstructural development in the weld deposit. It is suggested that the development of two different empirical carbon equivalent equations, one for very low carbon steels and one for general steels, has come about because of the different kinetic conditions that exist at low carbon concentrations, when a small change in carbon concentration leads to a large change in mechanical properties.

It is noted that increasing the volume fraction of \(\alpha_w\) in a weld at the expense of acicular ferrite is undesirable, since this is detrimental to toughness, and yet does not increase the strength of the weld.
REFERENCES


FURTHER PREDICTIONS ABOUT WELD METAL STRENGTH

6.1 INTRODUCTION

In general, when the volume fractions of the different phases are similar, a "rule of mixtures" is believed to be quite a good way of calculating strength (Ion et al., 1984; Ashby, 1987). Thus, it should be possible to model the yield strength of a weld as the sum of the products of the volume fractions of the three principal phases and their stresses at yielding. In fact, work showed that direct analysis of this sort on its own is inadequate, and does not give satisfactory results. This is because the composition of the alloy must also be taken into account.

In Chapter 5, it was shown that the strength of a weld can be factorised into components due to the intrinsic strength of iron, solid solution strengthening, and the contributions from the three major phases (\(\alpha, \alpha_w, \alpha_a\)) which constitute the microstructure, i.e.

\[
\sigma_y = \sigma_{Fe} + \sum_{i=1}^{k} \sigma_{SS_i} + \sigma_\alpha v_\alpha + \sigma_a v_a + \sigma_w v_w
\] (6.1)

where \(\sigma_{Fe}\) is the strength of fully annealed pure iron as a function of temperature and strain rate,

\(\sigma_{SS_i}\) is the solid solution strengthening due to an alloying element \(i\),

and \(\sigma_\alpha, \sigma_a, \) and \(\sigma_w\) are the microstructural strength contributions, and \(v_\alpha, v_a,\) and \(v_w\) are the volume fractions of the allotriomorphic, acicular, and Widmanstätten ferrite phases respectively.

This work is concerned with the further validation and development of this model, and involves the examination of a much larger number of welds. The ability to predict strength as a function of temperature is also investigated in this chapter.
6.2 EXPERIMENTAL METHOD

To test this model, three low-carbon manganese multipass welds were fabricated from 20mm thick plate using the manual-metal-arc welding process according to ISO-2560-1973 specifications. An ISO-2560 specification was used, since it is a joint geometry that leaves much of the weld metal free from dilution by the parent plate. The welding voltage was 23V (DC +ve) and a current of 180A was used. The net heat input was approximately 1.5 kJ/mm, and the maximum interpass temperature was 250°C. The welding speed was approximately 4 mm/s. The number of beads per weld was typically 25, each layer consisting of some three beads. The carbon content was manipulated using specially developed experimental electrodes, so that significantly different weld metal microstructures would evolve, the effect of increasing the carbon content being to increase the amount of acicular ferrite at the expense of allotriomorphic and Widmanstätten ferrite (Evans, 1981).

Weld metal chemical analyses are given in Table I.

<table>
<thead>
<tr>
<th>Weld ID</th>
<th>C</th>
<th>Mn</th>
<th>Si</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Ni</th>
<th>Mo</th>
<th>V</th>
<th>Ti</th>
<th>Al</th>
<th>N</th>
<th>O</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.1</td>
<td>0.043</td>
<td>1.25</td>
<td>0.43</td>
<td>0.017</td>
<td>0.008</td>
<td>0.02</td>
<td>0.02</td>
<td>0.005</td>
<td>0.002</td>
<td>0.010</td>
<td>0.002</td>
<td>72</td>
<td>394</td>
</tr>
<tr>
<td>6.2</td>
<td>0.10</td>
<td>1.56</td>
<td>0.42</td>
<td>0.015</td>
<td>0.007</td>
<td>0.04</td>
<td>0.04</td>
<td>0.01</td>
<td>0.006</td>
<td>0.013</td>
<td>0.015</td>
<td>119</td>
<td>262</td>
</tr>
<tr>
<td>6.3</td>
<td>0.15</td>
<td>1.57</td>
<td>0.45</td>
<td>0.012</td>
<td>0.007</td>
<td>0.04</td>
<td>0.03</td>
<td>0.01</td>
<td>0.008</td>
<td>0.014</td>
<td>0.015</td>
<td>96</td>
<td>193</td>
</tr>
</tbody>
</table>

Table 6.1: Weld metal analyses.

Figure 6.1 illustrates the welding procedure used, and shows the macrostructure of Weld 6.1.

Figures 6.2a and b contrast the as-welded and reheated regions. A trace of the original columnar morphology can still be seen. It can be seen that reheating changes the microstructure considerably. Subsequent passes, however, (Fig. 6.2c) have little obvious effect, although some slight increase in grain size was discernable. The amount of reheated weld metal was estimated by superimposing a grid of 6500 squares on it and then using areal analysis, and was found to be 54% (27% acicular ferrite), although the error associated with this estimate may be greater than is statistically implied because of the difficulty in distinguishing the as-welded and reheated regions (Gretoft and Svensson, 1986).
Figure 6.1: Weld 6.1: Cross-section of the weld deposit. Etchant: Ground and swab etched (unpolished) in ammonium thiosulphate.
Figure 6.2: (a) As-welded and, (b) reheated and (c) double normalised (i.e. twice reaustenitised) weld regions. Etchant: 2% Nital.
Vickers hardness measurements (10 kg) were carried out in both the columnar (top bead) and reheated regions of the welds. Ten indentations were made for each measurement. The volume fractions of the phases present in the primary microstructure (top bead) were determined at 250× magnification using a Swift point counter. 1000 points were taken for each specimen. Quantitative metallographic data are given in Table 6.2.

<table>
<thead>
<tr>
<th>Weld ID.</th>
<th>Hardness (HV10)</th>
<th>Volume Fractions</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Primary</td>
<td>Reheated</td>
</tr>
<tr>
<td>1</td>
<td>200</td>
<td>171</td>
</tr>
<tr>
<td>2</td>
<td>232</td>
<td>212</td>
</tr>
<tr>
<td>3</td>
<td>252</td>
<td>241</td>
</tr>
</tbody>
</table>

Table 6.2: Metallographic and hardness results for primary microstructure.

6.3 THE DETERMINATION OF YIELD STRESS FROM HARDNESS

A considerable amount of published work deals with the strength of multirun welds as a whole, whereas this work is concerned initially with just the primary microstructure for which property data other than hardnesses are not common. However, it is possible to estimate the yield strength of the primary weld microstructure from the hardness. For a rigid-plastic material indented by a Vickers indenter, the 0.2% offset yield strength is given by (Cahoon et al., 1971)

\[
\sigma_y = \left( \frac{H}{3} \right) (0.1)^{(m-2)}
\]  

where \(H\) is the hardness

and \(m\) is the Meyer's hardness coefficient.

It has been shown theoretically, and confirmed experimentally (Tabor, 1951), that

\[
n = m - 2
\]  

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where $n$ is the strain-hardening exponent for the material.

Therefore, combining Eqns. 6.2 and 6.3 gives

$$
\sigma_y = \left( \frac{H}{3} \right) (0.1)^n
$$  \hspace{1cm} (6.4)

$n$ is indicative of the material's ability to work-harden (e.g. for pure iron, $n = 0.31$ (Davies, 1978); for a low carbon annealed steel, $n = 0.26$ (Low and Garofalo, 1947)). For a severely cold-worked material $n$ may be taken as zero, when (Bowden and Tabor, 1964)

$$
\sigma_y \simeq \frac{H}{3}
$$  \hspace{1cm} (6.5)

This simple relationship was applied to see if it would allow weld metal yield strength to be predicted from hardness measurements, but was found to consistently overestimate the weld metal yield strength. This is because the as-welded microstructure still retains some work-hardenability, and thus Eqn. 6.4 should be used. In fact, empirical relationships between the hardness and yield strength already exist (Hart, 1975; Pargeter, 1978). However, as Pargeter (1978) noted, simple correlations between hardness and yield strength will necessarily be inaccurate, because of the complexity of weld metal behaviour in a hardness test. Also, the strain-hardening coefficient, $n$, will not be a fixed value, but will be influenced by the hardness of the weld metal itself. However, an estimate for $n$ as a function of microstructure could be made using the values obtained for $K$ and $n$ for the individual microstructural constituents in Chapter 5.

Let

$$
\sigma = K \varepsilon^n
$$  \hspace{1cm} (6.6)

Then

$$
\frac{\sigma_y}{\sigma_{UTS}} = \left( \frac{\varepsilon_y}{\varepsilon_{UTS}} \right)^n
$$  \hspace{1cm} (6.7)
which, employing the assumptions made earlier ($\varepsilon_y = 0.002$; $\varepsilon_{UTS} \equiv n$) becomes

$$\frac{\sigma_y}{\sigma_{UTS}} = n^{-n}(0.002)^n \quad (6.8)$$

$\sigma_y$ and $\sigma_{UTS}$ were determined from Eqn. 5.22.

$n$ was then found by solving Eqn. 6.8 iteratively using the Newton-Raphson technique (Kreyzig, 1972). An estimate of the strength of the weld from its hardness could then be made by substituting the value obtained into Eqn. 6.4.

The variation due to the change in the strength of pure iron, and the solid solution strengthening were then subtracted for each weld to give the strengthening due to microstructure. These calculations are summarised in Table 6.3. The hardnesses are high since it is the primary columnar region that is being considered.

<table>
<thead>
<tr>
<th>Weld ID</th>
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<th>$\sigma_y$ MPa</th>
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Table 6.3: Strength analysis of the primary weld microstructure.

From the results of Chapter 5, the strengthening due to allotriomorph ferrite is expected to be appreciably less than that of the Widmanstätten and acicular ferrite phases, which should have approximately similar strengths. Both have morphologies giving them a smaller effective grain size than allotriomorph ferrite. This is further suggested by the increase in hardness in Welds 6.1–3, which can be connected directly with the increase in the amounts of acicular ferrite in the welds (see Table 6.2). Thus, it is expected that $\sigma_\alpha$ will be less than both $\sigma_a$ and $\sigma_w$.

As an additional experiment, Welds 6.1, 6.2, and 6.3 were heat-treated at 700°C for 50 hours. This prolonged heat treatment would have the effect of annealing the microstructure, and so $\sigma_{micro}$ should be nearly zero. The heat-treated welds are designated with the suffix R. After the heat treatment, the hardnesses of the
specimens were as follows:

Weld 6.1R: 125 HV
Weld 6.2R: 136 HV
Weld 6.3R: 133 HV

The interpretation of these results is given below.

6.4 METHOD OF ANALYSIS

In order to calculate $\sigma_\alpha$, $\sigma_a$, and $\sigma_w$, the results from Table 6.3 were collated with data from 78 other welds from a variety of sources (Abson, 1978; Abson, 1982; Cunha et al., 1982; Bailey, 1985; McRobie and Knott, 1985; Lathabai and Stout, 1987; Thewlis, 1987), combining data for 15 submerged-arc and 19 manual-metal-arc welds (Abson, 1978; Abson, 1982; Cunha et al., 1982; McRobie and Knott, 1987), 7 flux-cored arc welds (Lathabai and Stout, 1987), and 37 triple arc submerged-arc welds (Bailey, 1985; Thewlis, 1987). For all the welds cited, their composition, the volume fractions of the microstructural constituents in the primary regions, and their hardness data are all available. The precise welding conditions used vary considerably—for example, the arc energies associated with the different techniques vary by more than an order of magnitude from 0.7kJ/mm Abson (1982) to 20kJ/mm (Bailey, 1985), and preheat temperatures vary from room temperature to 250°C—but these differences are reflected in the different microstructures that evolve. Idiomorphic ferrite, comprising typically <1%, in Abson (1982), was counted as allotriomorphic ferrite for the present work. It should be mentioned that in Cunha et al. (1982), Welds 3 and 4 were ignored since the stated volume fractions of the phases present did not add up to unity. Also, their definition of proeutectoid ferrite in the welds whose volume fractions were given, showed they, in fact, meant allotriomorphic ferrite, and it was treated as such.

Since $v_\alpha$, $v_a$, and $v_w$ are not independent $v_w$ was written as $(1 - v_\alpha - v_a)$ during the factorisation of the microstructure component of strength. $\sigma_{\text{micro}}$ could then be solved as:

$$\sigma_{\text{micro}} = x + y(v_\alpha) + z(v_a)$$  \hspace{1cm} (6.9)
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Table 6.4: Summarising the data used in the calculation of yield strength and solid solution strengthening as a function of microstructure.

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Contd. overleaf.
where \( x = \sigma_w \)

\[
y = (\sigma_\alpha - \sigma_w)
\]

and \( z = (\sigma_\alpha - \sigma_w) \)

\( x, y, \) and \( z \) were then found by linear regression of \( \sigma_{\text{micro}} \) against \( V_\alpha \) and \( V_a \) for the 81 welds (Draper and Smith, 1966). The regression analysis works to minimize the deviance of the data, where the deviance

\[
D = \sum_{i=1}^{k} [\sigma_{\text{micro}} - x - y(V_\alpha) - z(V_a)]^2 \quad (6.10)
\]

The overall method for determining \( \sigma_\alpha, \sigma_a, \) and \( \sigma_w \) is summarised in Figure 6.3. The hardness is used to calculate the yield strength, from which is subtracted the strength of pure iron, and solid solution strengthening to give \( \sigma_{\text{micro}}' \). Combining this with the volume fractions of the phases present allows \( \sigma_\alpha, \sigma_a, \) and \( \sigma_w \) to be calculated. Regression analysis was performed using the Royal Statistical Society’s GLIM† (Generalised Linear Interactive Modelling) software.

6.5 RESULTS

Eqn. 6.9 was solved to give (with standard errors):

\[
x = 325 \pm 30 \text{ MPa}
\]

\[
y = -317 \pm 68 \text{ MPa}
\]

and \( z = -0.19 \pm 29 \text{ MPa} \)

Eqn. 6.1 may therefore be written as:

† ©NAG Central Office, 7 Banbury Road, Oxford, U.K.

100
Figure 6.3: Flow diagram illustrating the steps involved in factorising the strength.
\[ \sigma_y = \sigma_{Fe} + \sum_{i=1}^{k} \sigma_{SS_i} + 8V_{\alpha} + 325V_{w} + 325V_{\alpha} \text{ MPa} \quad (6.11) \]

Figure 6.4 shows a comparison between the observed yield strengths of the primary microstructure against those predicted using Eqn. 6.11.

After 50 hours at 700°C, the microstructures of Welds 6.1R, 6.2R, and 6.3R all showed plain columnar grains containing inclusions. As an example, Figure 6.3 shows the microstructure of Weld 6.1 before and after heat treatment. In Figure 6.3b, the grains still retain their columnar morphology, but the as-deposited weld microstructure has recrystallized to leave a uniform microstructure within the grains. Thus, although there may be a small strengthening effect due to grain size, \( \sigma_{micro} \) should be rather small.

As with the other results, the strain-hardening exponents for the heat-treated specimens were calculated using Eqn. 6.8. (To calculate \( \sigma_{UTS} \), it was assumed that the heat-treated microstructures comprised 100% \( \alpha \). This assumption is fair, since at the yield stress, \( \sigma_{\alpha} \) is almost negligible, and allows an estimate of the ultimate tensile strengths of the annealed welds). \( \sigma_y \) has been taken as \( \sigma_{Fe} + \sum_{i=1}^{k} \sigma_{SS_i} \). The results of the calculation of the hardnesses of the welds are given in Table 6.4.

<table>
<thead>
<tr>
<th>Weld ID.</th>
<th>( \sigma_y/\text{MPa} )</th>
<th>VHN (Measured)</th>
<th>VHN (Calculated)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.1</td>
<td>362</td>
<td>125</td>
<td>129</td>
</tr>
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<td>6.2</td>
<td>389</td>
<td>136</td>
<td>137</td>
</tr>
<tr>
<td>6.3</td>
<td>383</td>
<td>133</td>
<td>135</td>
</tr>
</tbody>
</table>

Table 6.5: Measured and calculated values of the hardness of welds 6.1R-3R, re-heated at 700°C for 50 hours.

6.6 DISCUSSION

The values obtained for \( \sigma_{\alpha}, \sigma_w, \) and \( \sigma_{\alpha} \) at yield compare extremely favourably, and are internally consistent, with those obtained in Chapter 5 (c.f. Eqn. 5.21a). In this Chapter, a much greater number of welds have been analysed, and the results
Figure 6.4: Comparison of observed yield strength of primary microstructure and that calculated by Eqn. 6.11. (Correlation coefficient = 0.81).
Figures 6.5a and b: (a) Weld 6.1: As-deposited weld metal adjacent to the fusion boundary, and (b) Weld 6.1R: After 50 hours at 700°C.
obtained, shown in Figure 6.4, demonstrate that this method works for a wide range of welds, irrespective of the welding process variables used. It can be seen that in Figure 6.4 the measured strengths are higher than the predicted strengths for higher strength welds. The most probable reason for this is that the effect of the microphases becomes more significant at higher strengths, and they then contribute noticeably to the microstructure. Since the microphases are primarily martensitic, they impart hardness to the weld and so raise the apparent strength. Indeed, it is this behaviour which perhaps ultimately limits the accuracy of this model. It should be noted that although \( \sigma_w \) and \( \sigma_a \) were found to be the same in this analysis (Eqn. 6.11), they will have different hardesses, since their capacities to strain-harden are different. This is accounted for in Eqn. 6.4.

By adding back \( \sigma_{Fe} \), it is also possible to calculate the hardness of the individual phases in a hypothetical unalloyed weld using Eqn. 6.3. For \( \alpha \), \( \alpha_w \), and \( \alpha_a \), the hardesses are 86, 189 and 195 HV respectively, and are the minimum hardesses that would be found in welds of homogeneous allotriomorphic, Widmanstätten or acicular ferrite. These values are considerably less than values found elsewhere (Chaveriat et al., 1987), because the solid solution strengthening contribution has been removed.

The effect of annealing the welds for 50 hours at 700°C was to reduce \( \sigma_{micro} \) to a minimal value in each case. By taking the yield strength of the welds as being equal simply to the sum of the strength of pure annealed iron plus the solid solution strengthening due to alloying elements in the welds, it can be seen from Table 6.4 that it has been possible to predict the hardness of the annealed welds with extreme accuracy. This is a significant result, since, from the outset, one of the key aims of this work was to construct a model that would be able to describe weld metal strength as a function of thermal history, as well as composition, which is what has been done. It is interesting to note that, after annealing, Weld 6.2 possesses the highest strength, since microstructural strengthening is absent and it has the highest solid solution strengthening.

Now that a model has been constructed which allows weld metal strength to be calculated as a function of microstructure and heat treatment, this offers the possibility of being able to predict strength as a function of temperature, since it is now possible to calculate how the yield strength of pure iron, and the solid solution strengthening due to dilute alloying element additions varies with tem-
perature. This should be an exciting development, and is ultimately necessary to
resolve many of the inconsistencies current in weld metal testing procedures. For
example, although quality toughness tests are habitually carried out at a range of
temperatures down to $-60^\circ$C, tensile tests are nearly always carried out at room
temperature, even though the strength of a weld is temperature dependent. As
an illustration of this, Figure 6.6a shows how the strength of the annealed weld,
Weld 6.1R, will vary with temperature over the range 100-750K. This is done us-
ing the experimental data and methods cited in Chapter 5. The resultant change
in strength is complex because it is the summation of the individual effects of
iron, with the alloying element additions that is being displayed. Nevertheless, it
can be seen that with decreasing temperature, the yield strength of the weld in-
creases considerably. This can be attributed principally to an increase in the yield
strength of iron itself. Figures 6.6b, c, and d show variously how dilute additions
of manganese, silicon, and nickel will then alter the strength of the weld. At room
temperature and above, all three elements provide strengthening. However, at sub-
zero temperatures, manganese, and especially nickel, are able to provide softening
by disrupting the b.c.c. lattice so that dislocations lying in potential energy minima
can glide more easily, making slip easier, although the exact mechanism by which
this happens is not understood (Leslie, 1981). This behaviour makes them desir-
able alloying elements for low temperature applications. Nickel is also favourable
at low temperatures from the point of view of toughness, since it increases the
cleavage strength of ferrite (Jolley, 1968). A continuous representation of the effect
of nickel on the yield strength of Weld 6.1R in the range 100-600K is given in Figure
6.7. Note the marked softening that occurs at reduced temperatures when nickel is
present. In contrast, Figure 6.6c shows that silicon exhibits no real softening effect
except at low temperatures. This work, therefore, offers the possibility that alloys
could be designed specifically for the environments for which they are intended.

In fact, it is not yet possible to calculate how the yield strengths of *as-deposited*
welds vary with temperature, since the primary microstructure of a weld metal
contains a dislocation substructure (Tremlett *et al.*, 1961; Mandziej and Sleeswyk,
1987). This contributes to raise the strength of a weld above that of a steel of
equivalent composition, and will comprise a major part of the microstructural
strengthening component, $\sigma_{\text{micro}}$. Experimental work due to Whapham and Ed-
wards [cited as ref. 13 in Judson and McKeown (1981)] apparently found there
to be no difference in the dislocations densities of acicular ferrite, allotriomorphic
Figures 6.6a-d: Weld 6.1R: Calculation of the yield strength of annealed weld as a function of temperature. (a) As alloyed, and (b, c, and d) with manganese, silicon, and nickel additions respectively.
Figure 6.7: Weld 6.1R: The effect of increasing percentage nickel on the yield stress of an annealed weld as a function of temperature. (Ni: 0-2.5wt%; temperature: 100-600K; yield stress: 0-630MPa). The effect of adding nickel was calculated by interpolating experimental data due to Leslie (1972).
ferrite, and even the as-deposited and reheated regions of a weld examined in the TEM. The work cited is confidential, and so cannot be critically assessed. However, the results are extremely improbable. Microstructural strengthening is directly related to the dislocation density (Keh and Weissman, 1963), and the high values obtained for $\sigma_w$ and $\sigma_a$ in the preceding analysis, relative to $\sigma_\ell$, reflect in part the different dislocation densities found in the three phases. Widmanstätten ferrite and acicular ferrite grow by displacive transformation, and so will tend to have a higher dislocation density than allotriomorphic ferrite, which grows diffusionally (Bhadeshia et al., 1985). In fact, acicular ferrite has indeed been found to have a relatively high dislocation density, of the order of $10^{14} \text{m}^{-2}$ (Yang, 1987), conducive with this transformation mechanism. Since a decrease in the temperature of a steel will cause a decrease in dislocation mobility (Maekawa, 1972), it is evident that the microstructural contribution of the phases present to the overall strength of a weld metal will be temperature dependent. This will lead to a more pronounced increase in strength with decreasing temperature than with solid-solution-strengthened iron. Thus, the present work may be seen to provide a lower bound for predicting how the yield stress of a weld, of equal strength at room temperature, would alter with decreasing temperature.

As well as primary weld regions, multirun weld deposits contain areas of reheated microstructure. Since these regions should have a similar hardenability to the regions containing the primary microstructure, we would expect the hardness of the reheated regions to reflect that of the primary microstructure. Figure 6.8 shows results from Table 6.3 combined with data given in Abson (1982) and Cunha et al. (1982), and it can be seen that this is indeed the case. The offset along the $x$ axis arises because the reheated regions will be consistently softer than the as-deposited regions. Recently, work, following on from this research, has been underway to predict the strength of multirun welds (Svensson et al., 1988). This has been done by treating the microstructure as comprising reheated and as-deposited regions which contribute different amounts towards the overall weld metal strength. Although this method is approximate, it has, so far, produced reasonable quantitative results.

6.7 SUMMARY

Using published data for the hardnesses of the as-deposited regions of steel welds, together with data from three experimental welds, coefficients for the microstruc-
Figure 6.8: Comparing the hardnesses of the primary and reheated microstructures.
(Correlation coefficient = 0.90.)
atural strengthening due to allotriomorphic ferrite, Widmanstätten ferrite, and acicular ferrite have been derived which are consistent with those obtained in Chapter 5, and confirm the model described above. This work also demonstrates that the yield strength of the primary microstructure of a weld can be estimated realistically from a knowledge of the volume fractions of the phases present, which are used to estimate the strain-hardenability of the weld metal, and its hardness.

Prolonged subcritical annealing of the three experimental welds, was found to remove the strengthening due to the as-deposited microstructure, the residual strength being found to be equal to the strength of pure annealed iron together with the solid solution strengthening due to the substitutional alloying elements present in the welds. Calculations of the effect of temperature on the strength of one of the welds revealed that at, and above, room temperature, manganese, silicon, and nickel additions all imparted strengthening. However, at low temperatures, softening was observed to occur with additions of nickel, and, to a lesser extent, with manganese and silicon additions, when these elements assist, rather than impede, slip. This work suggests, therefore, that additions of nickel are desirable to promote good mechanical strengthening in welds which are to be used at low temperatures. The possibilities of being able to predict quantitatively the as-welded yield strength of steel weld metals as a function of temperature, and the yield strength of multirun welds were also discussed.
REFERENCES


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CHAPTER 7

THE PREDICTION OF NON-UNIFORM ELONGATION

7.1 INTRODUCTION

The ductility of a metal is a measure of its ability to deform plastically without failure, and it is one of the most important parameters used to describe the mechanical behaviour of materials. In welding, it is conventional to specify minimum levels of required ductility for safe performance of the welded structure. Since the ability of a weldment to serve the purpose for which it was fabricated requires strict control of its mechanical properties, any systematic study of the factors which determine weld metal properties must include an investigation into the factors controlling their ductility. This work is of increased interest, since it was demonstrated in Chapter 5 how the true stress/true strain curve may be estimated for as-deposited microstructures up to the ultimate tensile strength.

The ductility of a specimen elongated in a tensile test is conventionally measured in two ways; from the engineering strain at fracture, $\epsilon_f$, (usually called the elongation), and the reduction in area at fracture, both usually expressed as a percentage. However, a major problem in analysing these two parameters, as Dieter (1976) pointed out, is that the occurrence of necking in the tension test makes any quantitative conversion between the two measures impossible. Separate treatments are, therefore, necessary.

The detailed characteristics of ductile failure in steel welds are a consequence of the presence of inclusions in the material which act as stress concentrators, and it is now recognized that the size distribution of inclusions in weld metals is an important factor in determining their properties (Cochrane and Kirkwood, 1979; Savage, 1980). Likewise, other details of the inclusion population are increasingly being highlighted as being influential on the mechanical properties of weld metals (Abson and Pargeter, 1986; Dowling et al., 1986; Shehata et al., 1987). It is expected, therefore, that the volume fraction of inclusions will be a critical parameter for ductility. However, in order to provide a general quantitative description of the ductile behaviour of weld metals, it will also be necessary to consider other
factors, such as the influence of the state of stress and strain in the material, and
the work-hardening properties of the metal (Teirlinck et al., 1988). This work aims
to identify the main factors that influence the engineering properties of elongation
and reduction in area in weld metals, and to provide models by which they may be
predicted. Whilst a limited amount of work has been done on modelling the ductile
failure of steel weld metals (Hill and Passoja, 1974; Farrar, 1976; Roberts et al.,
1982), research has concentrated on the properties of weld metals under impact,
rather than under uniaxial tensile loading. This chapter, and the one following,
aim to show that elongation and reduction in area are dependent upon different
parameters, and describe different aspects of materials behaviour; simple models
are presented to describe them.

7.2 THE STRESS-STRAIN CURVE

The engineering tension test is used widely as an experimental technique by which
the mechanical properties of a material may be evaluated, and also as a standard
test by which the quality of a material may be adjudged. It involves a specimen
being subjected to a continually increasing uniaxial load, whilst simultaneously the
elongation of the specimen is recorded. An engineering stress-strain curve can then
be constructed from the load-elongation measurements made on the test specimen.
The engineering stress is a measure of the average longitudinal stress in the tensile
specimen, and is obtained by dividing the load at a given point by the original
cross-sectional area of the specimen. Similarly, the engineering strain, \( e \), is the
average linear strain, and is obtained by dividing elongation of the initial gauge
length of the specimen, \( \Delta l \), by its original length, \( l_0 \) (Dieter, 1976). This gives

\[
e = \frac{\Delta l}{l_0} = \frac{l - l_0}{l_0}
\]  

(7.1)

where \( l \) is the gauge length.

Figure 7.1 shows a typical engineering stress-strain tensile test curve. In the
elastic region up to the yield stress, stress is linearly related to strain by the Young's
modulus. When the yield stress is exceeded the specimen undergoes gross plastic
deformation. Then, as the metal work-hardens, the stress to produce continued
plastic deformation increases with increasing strain, and the strain is accommo-
dated uniformly throughout the specimen. During this period the volume remains essentially constant, and as the specimen lengthens it decreases uniformly across the gauge length in cross-sectional area. The flow curve of many metals in the region of uniform plastic deformation can be expressed empirically by the simple power law curve relation due to Nadai (1931):

$$\sigma = K\epsilon^n$$  \hspace{1cm} (7.2)

where $\epsilon$ is the true strain

\[ n \] is the strain hardening exponent

and $K$ is the strength coefficient, equal to the value of the flow stress at $\epsilon^n = 1.0$.

This equation describes a state of stable yielding, and, although a number of alternative equations exist, it is this equation which has been most successfully applied by various workers in describing weld metal tensile behaviour in this regime (Tweed, 1983; McRobie and Knott, 1985).

Eventually a point is reached where the decrease in area is greater than can be supported by the increase in deformation load arising from strain hardening. The maximum stress associated with this point is the ultimate tensile strength, $\sigma_{UTS}$, and the strain at maximum load up to which the cross-sectional area decreases uniformly along the gauge length, is the uniform elongation, $\epsilon_u$. Following the UTS, an instability will be reached at a point in the specimen that is slightly weaker than the rest. Further plastic deformation is concentrated in this region, and the specimen begins to neck down locally. The onset of necking may be defined by the Considère construction (Considère, 1885). Plastic deformation during necking is confined to the necked region, and the applied load continues to drop until the specimen fractures. This is illustrated in Figure 7.2. For steels, beyond necking, the true stress-strain curve is almost linear to fracture (Le Roy et al., 1981). It is important to observe that once necking occurs, the constraints produced by the non-deforming region outside the neck produce a state of triaxial stress in the neck. Thus, the average stress required to cause flow from maximum load to fracture is higher than would be required if only uniaxial stress were present. Eventually the specimen fails by strain under conditions approaching plane strain to give the cone part of a typical 'cup and cone' fracture (Rogers, 1960; Bluhm and Morrissey, 1966).
This fracture effectively takes place by internal necking of the matrix material.

The true strain during testing is defined as follows:

$$\varepsilon_L = \ln \left( \frac{l}{l_0} \right)$$

(7.3)

In this work, the subscripts L and A will be used to differentiate explicitly between strain calculated from change in length, and strain calculated from change in cross-sectional area respectively.

This equation is only applicable to the onset of necking while there is a homogeneous distribution of strain along the gauge length of the tensile specimen. Beyond maximum load, the true strain should be based on measurements of the actual area ($A$) or diameter ($D$), when

$$\varepsilon_A = \ln \left( \frac{A_0}{A} \right)$$

$$= 2 \ln \left( \frac{D_0}{D} \right)$$

(7.4)

### 7.3 The Factors Controlling Ductility

Ductile failure commonly occurs progressively, with void or crack nucleation at inclusions or particles, the growth of these voids with increasing plastic strain, and finally coalescence of the voids. Thus, it follows that the presence of particles in the microstructure can markedly affect ductility. Void coalescence occurs in the centre of the specimen. The central crack grows rapidly to complete fracture by the continued linking of voids as the applied load is accommodated by steadily fewer ligaments of matrix. Final separation occurs as the result of intense shear between voids.

Any discontinuity such as an inclusion in a material will cause a disturbance of a uniform applied stress field. Having nucleated voids of particles, the holes then
<table>
<thead>
<tr>
<th>Shape of Specimen</th>
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</thead>
<tbody>
<tr>
<td></td>
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</tr>
<tr>
<td></td>
<td>Other</td>
</tr>
<tr>
<td>Particles</td>
<td>Volume fraction</td>
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<tr>
<td>Type of particle</td>
<td>Inclusion</td>
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<tr>
<td></td>
<td>Dispersion</td>
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<tr>
<td></td>
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</tr>
<tr>
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<tr>
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<td>Matrix</td>
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<td>Spacing between particles</td>
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<td></td>
<td>Orientation</td>
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<td>Yield stress</td>
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<td>Flow stress</td>
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<td>Fracture stress</td>
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<td>Dislocation cell structure</td>
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<tr>
<td></td>
<td>Deformation mode due to stacking fault energy</td>
</tr>
</tbody>
</table>

grow as the applied tensile strain increases until they coalesce to give a fracture path (Fig. 7.3). Because of its stress-concentrating effect, a spherical void will elongate initially at a rate of about twice that of the specimen itself. As it extends and becomes ellipsoidal, however, it grows more slowly until, when very elongated, it extends at the same rate as the specimen itself (Martin, 1980).

Criteria for ductile fracture must take into account the fact that these different processes are involved and the parameters controlling them. The factors that can affect the ductility of a given material are given in Table 7.1 overleaf. The main variables are yield stress and the work hardening rate of the matrix, the cohesion of the matrix/particle interface, the size and shape of the second phase particles, their hardness, their volume fraction and their number per unit volume. Inevitably, in such a complicated situation, criteria for ductile fracture give weight to only a few of these factors, and will tend, therefore, to be applicable only to certain situations, but experience suggests that the work-hardening characteristics of the matrix material, and the nature of the inclusion population are the main causal factors in determining the true strain experienced during non-uniform deformation.

Percent elongation is primarily dependent upon the physico-mechanical properties of the material, and will be a function of the capacity of the material to work-harden. However, a complication in modelling elongation is that, since an appreciable fraction of the deformation will be concentrated in the necked region of the specimen, the value of $e_f$, the final total strain, will depend on the gauge length, $l_o$, over which the measurement is taken. The smaller the value of $l_o$, over which the measurement is taken, the greater the contribution from the neck and the higher the value of $e_f$. This gauge length dependence must also be accounted for. In fact, because percent elongation and percent reduction in area are both dependent upon specimen geometry and deformation behaviour they should not be taken unreservedly as true material properties. Nevertheless, they are valuable, widely used, guides to ductility, and useful in detecting quality changes in weld metals.

The factors that control the observed values for reduction in area are discussed in detail in Chapter 8.
Figure 7.3: Macroscopic central cavity formed in neck of copper tensile specimen immediately prior to fracture. The final shear stage of separation has started (at A). (After Groom, J. D. G. (1971), Ph.D. thesis, University of Cambridge, U.K., Chapter 1).
7.4 EXPERIMENTAL METHOD

An experiment was designed in order to see how ductility varies for weld metal with the same composition, and inclusion population, but with different matrix strengths. To do this, tensile testing was carried out on a series of welds at a variety of temperatures, so that different strengths would be exhibited.

Five low-carbon manganese multipass welds were fabricated to give welds of approximately constant chemical composition. The joint geometry was in accordance with ISO 2560-1973 specifications. The number of weld runs was 23 or more, with three runs deposited per layer. The current and voltage used were 180A and 23V (DC positive) respectively. The net heat input was approximately 1.5 kJ/mm, and the maximum interpass temperature was 250°C. The nominal plate and deposit composition were Fe-0.12C-0.55Mn-0.25Si wt%, and Fe-0.07C-1.2Mn-0.05Si wt% respectively. The number of beads per weld was usually 25, and not less than 23. The weld metal compositions are given in Table 7.2.

<table>
<thead>
<tr>
<th>Weld No.</th>
<th>C</th>
<th>Mn</th>
<th>Si</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Ni</th>
<th>Mo</th>
<th>V</th>
<th>Ti</th>
<th>Al</th>
<th>N</th>
<th>O</th>
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<td>1.28</td>
<td>0.44</td>
<td>0.019</td>
<td>0.008</td>
<td>0.05</td>
<td>0.01</td>
<td>0.008</td>
<td>0.009</td>
<td>0.005</td>
<td>85</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.2</td>
<td>0.060</td>
<td>1.31</td>
<td>0.44</td>
<td>0.018</td>
<td>0.008</td>
<td>0.06</td>
<td>0.01</td>
<td>0.006</td>
<td>0.008</td>
<td>0.014</td>
<td>97</td>
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<td>0.008</td>
<td>0.004</td>
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</table>

Table 7.2: Weld metal analyses.

Two all-weld metal tensile specimens, threaded at each end, with cylindrical gauge lengths were extracted longitudinally and machined from each weld in accordance with SMS 674-10C50 specifications to give five pairs of tensile specimens in all, although, because of the limited amount of weld metal available, four of the specimens could only be made with a gauge length of 55mm instead of the recommended 70mm. The specimens were degassed for 16 hours at 250°C to remove hydrogen prior to testing. By testing at more than one temperature, this work would also complement the work described in Chapter 5 when a computer program was written depicting the effect of temperature on the strength of iron.
and solid solution strengthening of alloying elements in iron.

Tensile testing was carried out in situ at ambient temperature, 0, -20, -40 and -60°C, the temperatures being achieved using mixtures of dry-ice and alcohol. The strain rate was approximately \(2 \times 10^{-4}/s\). The tensile specimens were threaded into place, and then a Pt thermocouple was taped to each specimen prior to testing to ensure that the appropriate temperature was attained, although during testing the temperature recorded unavoidably rose an average of 8.5°C as a consequence of deformation-induced heat evolution.

### 7.5 RESULTS

Tensile testing results are given in Table 7.3. \(\sigma_y\) is the yield strength, and \(\sigma_{UTS}\) is the ultimate tensile strength. The elongation and reduction in area at fracture have been designated EL and \(q\) respectively. Figure 7.4 shows that tensile failure occurred by a ductile ‘cup and cone’ mechanism.

<table>
<thead>
<tr>
<th>Weld No.</th>
<th>T/K</th>
<th>(\sigma_y/\text{MPa})</th>
<th>(\sigma_{UTS}/\text{MPa})</th>
<th>(\sigma_y/\sigma_{UTS})</th>
<th>EL (%) on 70mm</th>
<th>q (%) on 55mm</th>
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</thead>
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<tr>
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<td>297</td>
<td>522</td>
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<td>-</td>
</tr>
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<td>273</td>
<td>506</td>
<td>571</td>
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<td>-</td>
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<td>0.933</td>
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<td>27.8</td>
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<td>571</td>
<td>619</td>
<td>0.922</td>
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<td>30.8</td>
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</tbody>
</table>

Table 7.3: Welds 1–5: Results for mechanical testing results, carried out at temperature T.

During tensile testing, plastic deformation will be accommodated in the tensile
Figure 7.4: End-on view of the two halves of a tensile test specimen (Weld 1A) showing 'cup and cone' fracture (×15).
specimen. Elastic extension, however, will occur in both the specimen and the tensile testing machine, thus making the actual elongation, as determined from load-extension curves, appear larger than it actually is. This behaviour can lead to errors in estimates of Young's modulus of up to 2 orders in magnitude (Thompson, 1988). It was found that elastic stretching of the machine caused the gradient of the elastic line on the stress-strain curves, which should have a value of the modulus of elasticity for the material, to be only $\frac{1}{10}$ of its expected value. Accordingly, the components of elastic strain and plastic strain, $\epsilon_e$ and $\epsilon_p$, were calculated separately.

The elastic extension, $\Delta l_e$, has been calculated from Young's modulus, $E$. The modulus of elasticity for a material, as determined at ambient temperature, is extremely structure insensitive, and only slightly affected by changes in composition. For low-alloy steel weld metal, $E \approx 207$ GPa (Dieter, 1976). Therefore, from the definition of Young's modulus

$$\Delta l_e = \frac{\sigma l_o}{E} \quad (7.5)$$

where $\sigma$ is the average stress on the material.

Therefore

$$\Delta l_e = \frac{F}{E} \times \frac{l_o}{A} \quad (7.6)$$

where $F$ is the applied load.

$A$ has been calculated as follows. Since the reduction in area before the UTS is reached occurs uniformly along the specimen then, at any given time, assuming constant volume,

$$A_o l_o = A l$$

$$= A(l_o + \Delta l_p + \Delta l_e)$$

for which $\Delta l_p$ is the plastic extension of the specimen.

Therefore
It follows, from Eqn. 7.6,

\[ \frac{l_0}{A} = \frac{1}{A_0} (l_0 + \Delta l_p + \Delta l_e) \quad (7.7) \]

\[ \Delta l_e = \frac{F}{EA_0} (l_0 + \Delta l_p + \Delta l_e) \quad (7.8) \]

Therefore

\[ \Delta l_e EA_0 - F \Delta l_e = F (l_0 + \Delta l_p) \]

which leads to

\[ \Delta l_e = \frac{F (l_0 + \Delta l_p)}{EA_0 - F} \quad (7.9) \]

The extension due to plastic deformation, \( \Delta l_p \), is read directly from the load-extension curve, as shown in Figure 7.5. The elastic and plastic elongations, and plastic strain experienced by the specimens during tensile testing are given in Table 7.4. \( F_{UTS} \) is the applied load at the UTS, \( \Delta l_{ue} \) and \( \Delta l_{up} \) are the elastic and plastic extensions achieved during uniform elongation, \( \Delta l_{up}^{Total} \) is the total uniform elongation, and \( \epsilon_{up} \) is the value of the uniform plastic strain for the welds tested.

The total uniform plastic strain, \( \epsilon_{up} \), corresponds, therefore, to the total strain up to the ultimate tensile strength, since the elastic component is relieved at fracture.

Although elongation varied with temperature, Figures 7.6a and b show that for the temperature range investigated, reduction in area did not change.†

† It would be misleading to try to relate percent elongation and temperature from the data recorded, since elongation is a function of gauge length and the specimens used were not of identical geometry.
Figure 7.5: Illustrating the distinction between the elastic and plastic components of a load-elongation curve.
Table 7.4: Calculation of plastic strain for Welds 7.1–7.5.

### 7.6 DISCUSSION

The extension of a specimen at fracture can be expressed according to the expression due to Barba (1880):

\[
l_f - l_o = \alpha + e_{ul} l_o
\]

where \(l_f\) is the final gauge length of the specimen,

\(\alpha\) is the local necking extension,

and \(e_{ul} l_o\) is the uniform extension of the specimen.

This gives

\[
e_f = \frac{\alpha}{l_o} + e_{ul}
\]

The local necking extension, \(\alpha = \beta \sqrt{A_o}\). Therefore, from Barba's law, the
Figures 7.6a and b: (a) Reduction in area, and (b) ultimate tensile strength as a function of temperature for the experimental welds.
elongation:

\[ e_{fl} = \beta \frac{\sqrt{A_c}}{l_o} + e_{ul} \]  \hspace{1cm} (7.12)

where \( \beta \) is a constant of proportionality (Unwin, 1903).

Although \( \beta \) is taken as constant in a weld metal, it could be expected to be a function of the inclusion content, and so, indirectly, the amount of oxygen, sulphur, &c., in the weld, since the extent of non-uniform deformation must depend on these factors.

Eqn. 7.12 clearly shows that the total elongation is a function of the specimen gauge length, and, therefore, to compare elongation measurements of different sized specimens the specimens must be geometrically similar, i.e. for round bars \( \frac{L}{D_o} \) should be fixed. In this analysis, data due to Widgery (1974; 1976) have been used. Widgery carried out mechanical tests on a large series of GMAW low-alloy steel welds. This work was particularly interesting because it included a detailed examination of the inclusion populations of 16 welds. More importantly, the maximum uniform strain achieved by each specimen in the course of tensile testing, \( \epsilon_u \), was also recorded. Figure 7.7 shows the relationship between measured elongation, \( EL \), and ultimate tensile strength, \( \sigma_{UTS} \), for Widgery's welds. It can be seen that the recorded elongation decreases as the readiness of the weld metal to deform, as indicated by \( \sigma_{UTS} \), increases.

Since \( e_{ul} = \frac{l_u - l_o}{l_o} \)

then \( \epsilon_{ul} = \ln(1 + e_{ul}) \)

and \( \epsilon_{ul} = \{\exp(\epsilon_{ul}) - 1\} \)  \hspace{1cm} (7.13)*

Therefore \( \% \) Elongation = \( e_{fl} \times 100 \)
Figure 7.7: Showing the dependence of weld metal elongation on ultimate tensile strength. Data are due to Widgery (1976).
<table>
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<tr>
<th>Weld No.</th>
<th>$\beta \sqrt{\frac{A_o}{l_o}}$</th>
<th>$\epsilon_{u_L}$ (Max)*</th>
<th>$\epsilon_{f_L}$ (Calculated)</th>
<th>EL (%) (Measured)</th>
<th>EL (%) (Calculated)</th>
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<tbody>
<tr>
<td>7.1A</td>
<td>0.0937</td>
<td>0.146</td>
<td>0.242</td>
<td>26.8</td>
<td>24.2</td>
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<tr>
<td>7.1B</td>
<td>0.118</td>
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<td>0.265</td>
<td>28.8</td>
<td>26.5</td>
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<tr>
<td>7.2A</td>
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</tr>
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<tr>
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<td>26.5</td>
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* Maximum uniform plastic strain.

Table 7.5: Measured and calculated values of percent elongation for the weld metal tensile specimens.

\[ = \left\{ \beta \sqrt{\frac{A_o}{l_o}} + \exp (\epsilon_{u_L}) - 1 \right\} \times 100 \quad (7.14) \]

It should be emphasized that $\epsilon_{u_L}$ is expected to be very closely related to the work-hardening coefficient, $n$ (see e.g. Davies, 1978). Widgery (1974) found the two to be heavily correlated, with the best fit line: $n = 0.024 + 0.65 \epsilon_{u_L}$. $\beta$ is dependent upon alloy microstructure and composition, but for low-alloy steels, $\beta$ has a characteristic value of 0.73 (Lessels, 1954), and this was the value taken for the moment.

Figure 7.8 plots calculated and measured values of percent elongation for the experimental welds using data from Table 7.5. For Widgery's experiments, subsize specimens were used, but of recommended British standard dimensions (Lessels, 1954). The diameter and length were 8.41mm and 22.7mm respectively, \( \frac{l_o}{D_o} = \)

* Engineering strain, $\epsilon$, and true strain, $\epsilon$, are essentially identical for strains less than 0.1, but for higher strains $\epsilon$ is less than $\epsilon$.  

---
Figure 7.8: Calculated and measured values of percent elongation for the experimental welds (see Table 7.5).
Table 7.6 lists the maximum uniform strain achieved, together with measured and calculated values for elongation, EL, and reduction in area at fracture, q. Figure 7.9 plots calculated and measured values of percent elongation for Widgery's welds. The fair agreement between theory and experiment implies the necking process contributes a fixed amount to the elongation. However, it can be seen that the graph does not concur with the data in Figure 7.8, even though both sets of data are internally consistent. The explanation for this is that $\beta = 0.73$ applies to low-alloy wrought steels. However, because weld metals contain inclusions, not only will $\beta$ tend to be smaller (since the amount of elongation by the specimen after the UTS will be reduced), but the value of $\beta$ should correlate with the volume fraction of inclusions. The inclusion fraction, I, in volume %, may be evaluated using the approximate relationship (Widgery, 1977; Abson et al., 1978; Widgery, 1979):

$$I \approx 5.5(wt\%[O] + wt\%[S]) \quad (7.15)$$

The best value for $\beta$ was found to be

$$\beta = 1.239 - 1.704 \times I = 1.239 - 9.372 \times (wt\%[O] + wt\%[S]) \quad (7.16)$$

For example, $I = 0.30$ vol% gives $\beta = 0.73$. However, for a larger volume fraction of 0.50 vol%, $\beta$ drops to 0.39. Table 7.7 gives new calculated values for percent elongation incorporating Eqn. 7.16 to give

$$\%\text{Elongation} = \{1.239 - 9.372 \times (wt\%[O] + wt\%[S])\} \times \frac{\sqrt{A_o}}{L_o} + \exp(\epsilon_{uL}) - 1 \times 100 \quad (7.17)$$

Calculated and measured values of percent elongation, EL, are plotted in Figure 7.10 for the experimental welds and for the data due to Widgery (1976). It
<table>
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<th>Weld</th>
<th>Maximum uniform strain, $\varepsilon_u$</th>
<th>EL (%)</th>
<th>ES (%)</th>
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</tr>
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</table>

Table 7.6: Calculation of percent elongation. (Welds given in Widgery (1976)).
Figure 7.9: Measured elongations for 30 welds plotted against elongations calculated using Equation 7.6.
can be seen that the differences in gradient observed in Figures 7.8 and 7.9 have disappeared, and that general agreement is much better.

7.7 SUMMARY

The factors that control weld metal elongation have been reviewed. Up to necking, deformation occurs evenly along the length of the tensile specimen. For this region of the stress-strain curve, a strong correlation was observed between percent elongation and the maximum uniform strain, \( \varepsilon_{UL} \), which in turn is related directly to the work-hardening characteristics of the weld metal. Since it is already possible to estimate the uniform component of elongation for as-welded microstructures (see Chapter 5), an attempt to relate \( \varepsilon_{UL} \) to the microstructure of multirun welds would be a suitable subject for future work, since this would then permit the prediction of weld metal strain to failure.

The strain experienced subsequent to necking is non-uniform, being dependent principally upon the inclusion size distribution, and volume fraction of inclusions in the weld deposit. It has been demonstrated that differences in measured elongation between sets of data for welds with known uniform elongations can be resolved in terms of differences in the volume fraction of inclusions in the weld metals, since they will influence the amount of local necking extension. A simple relationship has been arrived at, to allow the magnitude of this non-uniform contribution to be estimated for a given weld metal composition.

It has been found that the elongation of a weld metal tensile specimen can be predicted from a knowledge of the amount of the uniform elongation experienced during testing, (i.e. elongation up to the ultimate tensile strength), the chemical composition of the weld, and its geometry. This is done using a modified version of Barba’s law, when the two components of uniform and non-uniform lengthening are treated separately.

The strength of the matrix, for the range considered, has no influence on reduction in area which is predicted to depend heavily upon the characteristics of the inclusion population.
Figure 7.10: Recalculated and measured values for percent elongation for this work and for Widgery (1976), taking into account the inclusion population. The line of ideality, and 95% confidence limits are also drawn.
REFERENCES


<table>
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<tr>
<th>Weld No.</th>
<th>( [O] ) (wt%)</th>
<th>([S] ) (wt%)</th>
<th>( \epsilon_{uL} )</th>
<th>( \epsilon_{fL} )</th>
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Table 7.7: Recalculation of percent elongation for welds given in Tables 7.5 and 7.6.
CHAPTER 8

WELD METAL DUCTILITY: REDUCTION IN AREA

8.1 INTRODUCTION

It follows from the Chapter 7 that, except for very short gauge lengths, percent elongation is mainly influenced by uniform elongation, and is thus dependent upon the strain-hardening capacity of the matrix. In contrast, reduction in area is more a measure of the deformation required to produce fracture, and its chief contribution arises from the necking process. The work of Groom (1971) illustrates this. Groom studied the effects of various nominal prestrains on the behaviour of copper and steel tensile tests. Rolling and swageing were used to form embryonic voids. It was found that for all pre-strains, the reduction in area associated with necking alone was essentially constant (Fig. 8.1), showing that for a given inclusion spacing there is a critical level of triaxial tension that must be reached before fracture can occur by void coalescence and the "cup" stage of fracture can propagate. (The slight decrease at large prestrains can be attributed to the inclusion spacing being significantly reduced by large amounts of cold work, since it is the inclusion spacing in the plane through the minimum section of the neck that has to be considered). It is, therefore, correct to consider the uniform and non-uniform components of ductility, and their effects on elongation and reduction in area separately. In summary, therefore, the magnitude of $\varepsilon_u$, the uniform elongation, is a function of the strain hardening capacity of the material. In contrast, non-uniform elongation is expected to depend on the concentration and distribution of the stress-concentrating particles which influence deformation behaviour after necking.

8.2 STRESS INTENSIFICATION

The initial stress in the usual tensile test is uniaxial, so that load divided by reduced area gives the true stress. However, this procedure underestimates the peak stress after necking, since the necking process has triaxiality associated with it, as other components of stress are introduced (Dieter, 1968). The stress distribution in the neck of a tensile specimen consists of an axial tension which is uniform across the neck ($\sigma_t$), plus a hydrostatic tension ($\sigma_H$), which is zero on the periphery and
increases to a maximum on the axis. The effect of this variation of tension across the specimen is to make the mean stress ($\sigma_m$) higher than the true flow stress ($\sigma_t$). The correction factor was found by Bridgeman (1952) to be

$$\frac{\sigma_m}{\sigma_t} = \left(1 + \frac{2R}{a}\right) \ln \left(1 + \frac{a}{2R}\right) \quad (8.1)$$

where $a$ is minimum radius of the neck cross-section,

and $R$ is the radius of the neck profile (see Fig. 8.2).

This expression was derived using an approximate solution, based on a geometrical analysis of neck formation, and gives the best approximate procedure for obtaining the distribution of stresses and strains during ductile failure. Triaxiality will have a strong effect upon the rate of growth of a spherical void, and consequently upon the strain of fracture at a notch. Once the inclusion/matrix interface bond is broken, which is expected to occur early during testing, the superimposed triaxial stresses promote rapid void coalescence and enhance the 'cup' stage of fracture.

### 8.3 THE NECKING PROCESS AND REDUCTION IN AREA

During non-uniform elongation it is only the neck region that lengthens substantially. For this deformation process the weld metal is considered microstructurally homogeneous, insofar as the phases by now all have similar strengths (see above), and necking is attributed to variations in inclusion population in the specimen. It has already been discussed in Volume 1 that the microstructure of a weld metal is inhomogeneous. Essentially three main phases are present - allotriomorphic ferrite formed at the austenite grain boundaries, Widmanstätten ferrite, and acicular ferrite consisting of a non-parallel array of bainite plates. However, Tweed and Knott (1987) have shown by microhardness and Tolansky interferometry techniques that allotriomorphic ferrite, which is expected to be the softest of the three phases (Sugden and Bhadeshia, 1988), has preference of flow for the first 5-10% strain. Therefore, at higher strains, resistance to flow seems to be much the same in all three phases.
Figure 8.2: Triaxial stresses associated with tensile testing. \( P \) and \( A \) are the applied load and cross-sectional area of the specimen respectively. (After Marshall, E. R., and Shaw, M. C. (1952), *Trans. A.S.M.*, 44, 705-720).
The sequence of events that leads to ductile failure in a tensile test specimen can be summarised as follows (Rogers, 1960; Melander, 1981):

(i) voids form after a critical amount of strain;
(ii) at the maximum in the applied load, necking begins with further straining;
(iii) at a critical volume fraction of voids, or at a critical mean free path between voids, strain concentrates in narrow bands connecting the voids;
(iv) separation occurs along these bands.

Figure 8.3 shows the typical inclusion distribution in a low-alloy steel weld deposit.

In this part of the failure process, it is the void geometry that is most important. The overall strain, therefore, will strongly depend upon the inclusion spacing, failure being determined by a geometry criterion dependent upon the spacing of the void nucleating inclusions at the UTS.

The proportion of particles that form dimples (i.e. take part in the fracture process) in weld metals has sometimes been reported to be higher than the apparent inclusion density observed on a planar specimen (Tuliani et al., 1969; Siewert and McCowan, 1987), and Widgery and Knott (1978; 1980) interpreted this to mean that as internal necking occurs, inclusions beyond the plane of the specimen are drawn into the fracture of the specimen (Figure 8.4), such that the ratio of the depth from which a given inclusion is sampled, \( z \), to the diameter of the inclusion, \( x \), is constant. However, it should be mentioned that this is not a totally general result, and other particle-containing alloy systems exhibit different behaviours (Dodd and Bai, 1987, p.96).

An early investigation into the influence of inclusions on ductility was done by Edelson and Baldwin (1962) using copper-base alloys. Within experimental error, alloy ductility was found to be dependent upon the percent volume fraction of the inclusions present alone for \( V_f \) varying between 0 and 20% (see Figure 8.5). Similarly, Le Roy et al. (1981) found the strain to failure of spheroidized steels to decrease with increasing cementite volume fraction (Figure 8.6), and similar data are given in Pickering (1978). However, this relationship was tested for weld metals by Widgery (1976), and he found poor agreement. He considered that the yield
Figure 8.3: Low-carbon 2% nickel steel bead-on-plate weld deposit etched to reveal inclusions. Etchant: Acidified alcoholic CuCl₂.
Figure 8.4: Microvoid formation during ductile failure: only certain inclusions (solid circles in (a)) take part in the development of fracture (b). (After Widgery, D. J. and Knott, J. F. (1978), *Met. Sci.*, 12, (1), 9).
Figure 8.5: Combined plot of ductility of several copper dispersion alloys versus volume fraction. (After Edelson, B. I. and Baldwin, Jr., W. M. (1962), *Trans ASM*, 55, 230-250).
Figure 8.6: Strain to fracture in spheroidized carbon steels as a function of the percent volume fraction of cementite particles ($f_v$). ($\epsilon_n$ is a calculated void nucleation strain). The references on the diagram are given in the original reference. (After Le Roy, G., Embury, J. D., Edwards, G., and Ashby, M. F. (1981), Acta Metall., 29, 1509-1522).
strength and work-hardening characteristics of the matrix must also be important, and should be taken into account.

In order to see if weld metal ductility could be explained in terms of the volume fractions of inclusions present, data for reduction in area, $q$, and wt% oxygen were taken from the literature. Ductility, which may be taken as the strain to failure, is based in the reduction in area achieved during the tensile test as follows:

$$
\epsilon_{fA} = \ln \left( \frac{A_o}{A_f} \right) = \ln \left( \frac{100}{100 - \%RA} \right)
$$

where the subscript $A$ denotes that the strain has been calculated from the change in the cross-sectional area of the specimen during testing.

The amount of oxygen in the weld is directly related to the inclusion volume fraction (Pargeter, 1981).

Figure 8.7 plots ductility against wt% oxygen for 116 welds taken from the literature. The nature of the welding process used in each case is also indicated. Although higher ductilities appear to be associated with lower oxygen contents, there is no clear relationship between the two.

It is suggested that this is because

(i) in weld metals, the volume fraction of inclusions varies typically only in the narrow range from approximately 0.002 to 0.01 by weight,

and (ii) unlike the work due to Edelson and Baldwin (1962), and Le Roy et al. (1981), which used carefully controlled base metals, the matrix strength is not constant, and can vary quite considerably in a given set of welds.

In fact, it is possible to be more specific. The experimental results in Widgery (1974) contain data for the inclusion populations of 16 welds. Figure 8.8 illustrates how the non-uniform strain, ($\epsilon_{fA} - \epsilon_u$), calculated from his results, is strongly dependent upon the volume fraction of the inclusion present. It should be noted that for five of the welds (K, L, S, T, and U) the magnification of the image analyser that characterised the inclusion populations of the welds had been unreliably calibrated. Thus, the number of inclusions per mm$^2$, geometric mean inclusion diameter, and
Figure 8.7: The relationship between weld metal ductility and wt% oxygen. The welding process used is also recorded. The references used are cited below.


Figure 8.8: The relationship between necking strain and inclusion volume fraction, with 'best fit' line through solid points. \(\epsilon_f\) is the strain to failure, defined in Eqn. 8.2, \(\epsilon_u\) is the uniform reduction in area achieved during tensile testing. Therefore, \((\epsilon_f - \epsilon_u)\) represents the non-uniform strain attained during tensile testing. Data is taken from Widgery, (1974). (The accuracy of the hollow points is uncertain).
average nearest neighbour spacing might, or might not, be correct. Since the first
two parameters are needed in order to estimate the volume fraction of inclusions
present [according to the method due to Ashby and Ebeling (1966)], the values of
\( f_o \), and so the calculated values of reduction in area are questionable. Accordingly,
these points have been left hollow. These uncertainties were not mentioned when
the results were republished later (Widgery, 1976).

8.4 MODELS

Fracture research has led to a large number of increasingly sophisticated models
being formulated to help explain material behaviour quantitatively during ductile
failure. These have been the subject of a variety of excellent reviews (Goods and
Brown, 1979; Lagneborg, 1981; Embury, 1982; Dodd and Bai, 1987).

It is attractive to consider void coalescence as a gradual process involving the
thinning down of the ligaments between voids with increasing strain. Thus, fi-
nal separation occurs when the ligaments have reduced to zero width. However,
McClintock (1968) showed, using detailed calculations, that fracture strains an or-
der of magnitude greater than those observed experimentally are obtained when
void coalescence is taken to occur by this internal-necking mechanism. Thomason
(1968) modelled void linkage by considering a rigid/plastic material containing a
uniform distribution of square prismatic cavities. From this model it appears that
the total displacement between two surfaces that is necessary to cause coalescence
of cavities is approximately equal to their separation prior to coalescence. For most
materials he considers that the distance between adjacent cavities will be small at
this point. In a simpler adaptation of their model, Brown and Embury (1973)
hypothesized void linkage occurring by joining at an angle of 45°. However, this
model has been challenged recently by work due to Ellis (1987), who showed that
in a tensile test macroscopic necking will normally have occurred well before the
geometric condition is met.

An alternative approach to void coalescence is that fracture will occur when the
volume fraction of voids reaches a critical value that is characteristic of the material
(Rice and Tracey, 1969; Schmitt and Jalinier, 1982). Although, it is unclear what
the effect of the individual sizes of the voids would have, this approach looked
suitable for the general class of low-alloy steel weld metals, since it was seen in
Chapter 7 that \( \varepsilon_A \) does not appear to change for different matrix strengths. Particle
size alone does not appear to have any effect on ductility (Edelson and Baldwin, 1962). In this analysis, which aims to estimate $\epsilon_A$, the strain to failure, the model presented by Gurland and Plateau (1963), and Henry and Plateau (1967) has been used. It is presumed that not only is void growth proportional to macroscopic strain, but also that it is increased by the local strain concentration due to the largest curvature of the void. Void coalescence is then assumed to occur when a critical ratio of hole size in the direction of straining to the hole spacing is reached. This criterion was modified by Gladman et al. (1971; 1975) to give a critical ratio of inclusion diameter to ‘nearest neighbour’ spacing, implying a critical volume fraction of voids for coalescence. This enabled a simpler functional form for strain to failure to be derived.

Decohesion of the inclusion is presumed to occur at negligible strains, and this seems reasonable for weld metals. Widgery and Knott (1978) argued that if void nucleation strain were a critical parameter, it would depend upon inclusion size, in which case the inclusion size distribution on a microvoid fracture surface would both show a cut-off at low inclusion sizes, and also not correspond to the distribution measured on a carbon replica of an electropolished surface. These traits were not observed in their work on C-Mn weld metals, and it was concluded that no initiation strain is required, and that inclusions effectively act as voids.

The true strain to failure is given by the following equation:

$$
\epsilon_A = \frac{1}{2} \ln \left\{ \left( \frac{\phi^2}{f_o} + \frac{k}{r^2} \right)/(1 + \frac{k}{r^2}) \right\}
$$

(8.3)

where $\phi =$ critical volume fraction of voids, taken as 0.04,

$f_o =$ volume fraction of inclusions,

$k =$ a strain intensification factor,

and $r =$ the length-width ratio of the inclusion where straining is in the length direction (Lagneborg, 1981).

The inclusions are assumed to be spherical ($r = 1$), since they typically have a

† This equation was published incorrectly in Gladman et al. (1975).
higher melting point than steel, and therefore solidify in the weld before the steel. It is also assumed that the inclusions are elastically hard (non-deformable).

From Eqn. 8.2

$$
\varepsilon_{f_A} = \ln \left( \frac{100}{100 - \%q} \right)
$$

Therefore

$$
\%q = 100 - \frac{100}{\exp(\varepsilon_{f_L})}
$$

$$
= 100 - \frac{100}{\exp \left[ \frac{1}{2} \ln \left\{ \left( \frac{\phi^2}{f_s^2} + \frac{k}{r^2} \right)/(1 + \frac{k}{r^2}) \right\} \right]}
$$

$$
= \left[ 1 - \frac{1}{\sqrt{\left( \frac{\phi^2}{f_s^2} + \frac{k}{r^2} \right)/(1 + \frac{k}{r^2})}} \right] \times 100 \quad (8.4)
$$

$k$ was taken as 2 (Lagneborg, 1981).

Calculated and measured values of percent reduction in area for results due to Widgery (1974) are given in Table 8.1, and plotted in Figure 8.9.

Steel (1972) and Shehata (1987) performed tensile tests respectively on standard MMA and SA weld metal specimens for which the inclusion volume fractions had been determined experimentally. Table 8.2 gives experimental and calculated values for their welds. It should be emphasized that the welding processes used and the conditions of the welds are in contrast to each other. Steel used MMA as-deposited weld metal, whereas Shehata's was SA narrow-gap, post-weld heat treated. However, it should be noted that experimental evidence shows that the inclusion distribution will not be affected by PWHT (Tweed and Knott, 1983), and so the results of Shehata are perfectly admissible in this analysis. Results from Table 8.2 are plotted in Figure 8.10.
Figure 8.9: Measured and calculated values of percent reduction in area for Widgery (1974). (The hollow points are uncertain).
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Table 8.1: Measured and calculated values of percent reduction in area for Widgery (1974).

8.5 DISCUSSION

Figure 8.10 shows the good agreement that exists between the calculated and measured values of reduction in area obtained for the results of Steel (1972), and Shehata (1977). This indicates that, for a given class of materials, the Gladman equation provides a suitable model for the prediction of reduction in area, and that it can be predicted from the inclusion volume fraction.

For the results of Widgery (1974), shown in Figure 8.9, leaving aside the two unreliable points at the top of the graph, the points have a correlation coefficient of 0.75, indicating that the relationship is fundamentally correct. However, Eqn. 8.4 overestimates recorded values for reduction in area by a constant amount of ≈15%. Whilst there are many factors that might cause a discrepancy, such as differences
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<td>71</td>
<td>73</td>
</tr>
<tr>
<td></td>
<td>X17a</td>
<td>72</td>
<td>76</td>
</tr>
<tr>
<td></td>
<td>X17b</td>
<td>71</td>
<td>76</td>
</tr>
<tr>
<td></td>
<td>X11a</td>
<td>67</td>
<td>69</td>
</tr>
<tr>
<td></td>
<td>X11b</td>
<td>67</td>
<td>69</td>
</tr>
<tr>
<td></td>
<td>X18a</td>
<td>70</td>
<td>70</td>
</tr>
<tr>
<td></td>
<td>X18b</td>
<td>67</td>
<td>70</td>
</tr>
<tr>
<td></td>
<td>X19a</td>
<td>68</td>
<td>69</td>
</tr>
<tr>
<td></td>
<td>X19b</td>
<td>68</td>
<td>69</td>
</tr>
<tr>
<td></td>
<td>X12</td>
<td>47</td>
<td>63</td>
</tr>
<tr>
<td>Shehata (1987)</td>
<td>W1</td>
<td>74</td>
<td>85</td>
</tr>
<tr>
<td></td>
<td>W2</td>
<td>68</td>
<td>80</td>
</tr>
<tr>
<td></td>
<td>W3</td>
<td>70</td>
<td>82</td>
</tr>
<tr>
<td></td>
<td>W4</td>
<td>70</td>
<td>66</td>
</tr>
<tr>
<td></td>
<td>W5</td>
<td>70</td>
<td>69</td>
</tr>
<tr>
<td></td>
<td>A</td>
<td>75</td>
<td>84</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>70</td>
<td>85</td>
</tr>
</tbody>
</table>

Table 8.2: Measured and calculated values for percent reduction in area.
Figure 8.10: Measured and calculated values for percent reduction in area. (Data due to Steel (1972) and Shehata (1987)).
in the composition and hardness of the inclusions, differences in the experimental
techniques used for the analysis of the inclusion volume fractions, and differences in
the strengths and strain hardening behaviour of the welds, perhaps the most likely
cause is that Widgery's specimens were of unusually small dimensions ($l_0 < 25\text{mm}$).
The increased hydrostatic tensile stresses which arise as a consequence of necking
mean that the stress distribution across the tensile specimen is no longer planar,
and the average stress required to cause flow from maximum load is higher than if
only uniaxial stress were present. Ductility will tend to decrease in the presence of
a steep stress gradient and triaxial stress field. Since the latter is a function of the
test-piece dimensions, values of reduction in area are dependent upon specimen
geometry and dimensions (Dieter, 1968). There is a small effect of changes in
the strain-hardening exponent, $n$, during the process of void coalescence, and the
lower the value of $n$, the more rapidly voids will coalesce. However, this is thought
to be of secondary importance when compared with the effects of superimposed
triaxial stresses experienced in tensile testing. Thus, during the necking stage, when
triaxial stresses come into play, either the critical volume fraction of holes required
for failure, $\phi$, will be different, or, what appears more likely, the value of $k$, the
stress-intensification factor, will be different, for Widgery's smaller specimens. It
is, perhaps, significant, that the error between the calculated and predicted values
of percent reduction in area for Widgery's welds is constant, which suggests the
influence of a constant factor, such as specimen geometry.

Elongation is still predictable for Widgery's specimens (Chapter 7), since neck-
ing behaviour is not critical in this case.

8.6 SUMMARY

The parameters which determine weld metal reduction in area have been inves-
tigated. For a given set of welds, reduction in area is observed to decrease with
increasing volume fraction of inclusions. An even clearer correlation was observed
between the volume fraction of inclusions, and the post-UTS strain, indicating that
this is the part of the fracture process on which the inclusion population has most
influence.

A simple theory has been used to explain the adverse effects of inclusions on the
reduction in area of low-alloy steel weld metals. Fair agreement has been obtained
with results calculated from theory, and experimental data due to Steel (1972),
and Shehata (1987). Discrepancies between predicted and measured values for reduction in area for sub-size (geometrically similar) specimens have been tentatively attributed to differences in necking strain behaviour.
REFERENCES


CHAPTER 9

SCATTER IN WELD METAL TOUGHNESS MEASUREMENTS

9.1 INTRODUCTION

In conjunction with the other research described in this dissertation, work has also been underway to quantify the factors that determine weld metal toughness. Increasingly stringent mechanical property requirements are being imposed in the manufacture of ferritic steel constructions, and a detailed knowledge of the factors influencing weld metal toughness is consequently vital. The Charpy V-notch test is used widely in quality control for determining the toughness of steels. The test is empirical, but is popular because it is both uncomplicated and cheap to perform. In general, much less energy is required to propagate a cleavage crack in a steel than is necessary for a ductile crack to grow. This is demonstrable by carrying out impact tests over a range of temperature, when the energy absorbed by the specimen when plotted as a function of temperature usually shows a sigmoidal behaviour, as the mode of fracture changes from brittle to ductile (Figure 9.1). Though the absorbed energy measured in this test cannot be used directly in quantitative assessments of the resistance of structures to brittle fracture, it can be used in a comparative manner for quality control.

The problem of predicting the impact behaviour from a knowledge of microstructure as yet seems insurmountable, although there are certain aspects of toughness which correlate strongly with microstructure, and which seem to have a straightforward physical basis. It is clear from published data that the scatter in the measured toughness values obtained from weld metal toughness results is frequently much greater than that obtained when measuring the toughness of plain carbon steels of equivalent chemical composition (compare Figure 9.2), and it can be hypothesised that this might be connected with the constitution of the microstructure. This phenomenon has been commented on before. Neville (1985) observed that many materials show variation in the measured values of their toughness or resistance to catastrophic crack propagation, and, in his own work on ferritic steels, he noted that the introduction of microstructural inhomogeneities, such as hard pearlite islands, can lead to a significant variation in measured fracture tough-
Figure 9.1: Changes in Charpy V-notch properties for conventional pressure vessel steel plate, tested in the transverse (○) and longitudinal orientation (●) with respect to the rolling direction. (After Dieter, G. E. (1978), "ASM Metals Handbook", 8, 262).

Figure 9.2: Typical Charpy toughness results for Fe-0.03C-1.08Mn-0.55Si (wt%) multipass low-alloy steel MMA weld, characterised by a large degree of scatter (shaded region). (Data: courtesy B. Gretoft, ESAB AB).
ness values during repeat tests on specimens of the same material. Garland (1975a; 1975b) observed that erratic and occasionally low as-welded toughness results have been recorded in both laboratory tests and procedural trials on a range of structural steels despite using welding materials generally approved for critical fabrications at weld heat inputs typical for these applications. He recorded that the as-welded mechanical properties achieved cannot be reconciled with either weld metal composition, or weld metal microstructure, as conventionally assessed in terms of area fraction of the major microstructural constituents. Another reason, suggested by Hayes et al. (1986), is that in tests on narrow welds, the crack has been observed to deviate into the adjacent material giving high absorbed energy measurements, which reflect the yielding properties of the adjacent material, rather than the toughness of the weld metal. It is the aim of this work to show that this behaviour is a consequence of the inhomogeneity of weld metal microstructures.

Several workers have commented that specific regions in the microstructure of weld metals are potential sources of failure. For example, Mardziej and Sleeswyk (1987) found weld metals of almost identical chemical composition, produced by the same welding procedure and consumables, differed significantly in toughness values, and attributed this to regions of local brittleness in the microstructure. Similarly, Thaulow et al. (1987) carried out a detailed examination of the surfaces of failed SMA weld metal fracture toughness specimens. It was found that the majority of the brittle fractures in their specimens had initiated from the primary weld metal. Widgery (1972) also found that cleavage cracks initiate preferentially in the as-deposited microstructure of low-alloy steel weld metal. Thus, it appears that the different microstructural morphologies encountered in a weld metal do provide local regions of strength and weakness, and any assessment of the factors that affect weld metal toughness should, therefore, include an analysis of this behaviour.

This work is part of a continuing project which aims for the prediction of the mechanical properties of low-alloy steel weld deposits from a knowledge of their chemical composition and detailed fabrication history. The first part of this work aims to show that a large amount of the scatter obtained in weld metal toughness experiments can be attributed to the nonuniformity of the weld metal microstructure. Secondly, it is demonstrated that the mechanical properties of regions within multirun welds can be expected to vary locally.
9.2 ANALYSIS OF SCATTER

In order to try to interpret the broad scatter that may be obtained in the impact testing of weld metals, it was first necessary to find a suitable way of representing scatter. The three most frequently used ways of rationalising scatter in results from the toughness testing of weld metals are to take an average of the Charpy readings obtained at a given temperature (e.g. Evans, 1980), measure the standard deviation (Drury, 1984), or plot the lowest Charpy readings obtained to focus attention on the lower ends of the scatter bands (Taylor, 1982).

An alternative to this was suggested by Smith (1983) who proposed a Scatter Factor to quantify any spread obtained in Charpy values, where

\[
\text{Scatter Factor} = \frac{\text{Maximum energy} - \text{Minimum energy}}{\text{Average energy}} \times 100(\%) \quad (9.1)
\]

However, such an *ad hoc* relationship cannot be used to provide statistically meaningful results. Yet, a difficulty in being more specific is that we are attempting to describe the toughness of a weld metal over a range of temperature, rather than simply rationalise the scatter in a set of data at one temperature. The best way round this is first to fit a curve to a given set of data.

An idealised impact energy temperature curve is sigmoidal in shape, and the curve-fitting could be done by one of three ways:

(i) the least squares method which gives equal weight to all points,

(ii) a weighted least squares method,

or (iii) by fitting the data to a logistic (log-related) curve.

In fact, the last method is the most common for a sigmoidal, rather than plain curve, and appeared to be justified over an (unweighted) least squares analysis in that the residuals between the observed and fitted log/temperature scales (discussed below) were approximately the same at all temperatures, i.e. at steep and shallow gradients. A weighted least squares analysis was not attempted since there was no clear way by which the weighting could be applied.
The sigmoidal curve has the form (Bronshtein and Semendyayev, 1973):

\[
\ln\left(\frac{E}{E_{US} - E}\right) = \alpha + \beta T
\]  

(9.2)

where \(E\) = energy absorbed  
\(E_{US}\) = upper shelf energy  
\(T\) = temperature  

and \(\alpha\) and \(\beta\) are experimentally determined constants\(^\dagger\).

A difficulty with fitting the sigmoidal curve to the experimental data is that the upper shelf energy needs to be defined. For this analysis, \(E_{US}\) was taken to be 2% above the maximum recorded impact value. This treatment was found to be satisfactory, and is a fair assumption since the upper shelf energy is essentially independent of temperature over the range of interest (Honeycombe, 1981a). \(\alpha\) and \(\beta\) are determined by plotting the intercept and gradient respectively of a graph of \(\ln\left(\frac{E}{E_{US} - E}\right)\) against temperature.

Regression analysis was performed using GLIM (General Linear Interactive Modelling) software developed by the Royal Statistical Society. The optimum values for \(\alpha\) and \(\beta\) occur when the scatter of a given set of data points around a trial curve is a minimum. The scatter may be evaluated by calculating the deviance of the data, which is equal to the sum of the squares of the deviations of the sample observations from the mean. This may be expressed algebraically as

\[
\sum_{i=1}^{n} \left[ \ln\left(\frac{E_{i}}{E_{US} - E_{i}}\right) - (\alpha + \beta T_{i}) \right]^2
\]

The best values of \(\alpha\) and \(\beta\) are found, therefore, when this function is a minimum. However, in order to compare sets of data, it is necessary to consider the scale

\(^\dagger\)Perhaps the most common use of an equation of this form is in the quantitative description of reaction kinetics, \(e.g.\) Johnson and Mehl (1939)).
where $\nu$ is the number of degrees of freedom and illustrates the excess amount of data points available to be used in the regression analysis. It is defined as the number of data, $n$, minus the number of independent constraints on that set of data (Duckworth, 1968). The equation has two unknown constants, $\alpha$ and $\beta$, and so $\nu = (n - 2)$.

The scale parameter allows for the fact that the deviance of a large set of data will necessarily be greater than that of a smaller set of equally scattered data. The attraction of this method is that it quantifies scatter irrespective of the actual shape, and absolute magnitudes of the data, of the curve. It should be noted that this technique will give a false indication of the scatter associated with a given Charpy curve if only a few readings have been taken, and, irrespective of the proportions of various phases in the microstructure, if only three pairs of data are provided, the deviance will be zero! To guard against this, it is suggested that a minimum number of, say, ten readings per curve should be taken.

A computer listout of the program used for the evaluation of scatter is given in Appendix 6.

9.3 QUANTIFICATION OF HETEROGENEITY

Since it is believed that the variation in Charpy results obtained from similar welds at the same temperature depends upon the phases present in the weld, the inhomogeneity of a given weld metal microstructure would also need to be quantified. This was can be done by calculating the entropy, $H$, of a given microstructure (Large 1967; Karlin and Taylor, 1975).

Let $X$ be a random variable assuming the value $i$ with probability $p_i$, $i = 1, \ldots, n$. The entropy of $X$, as a logarithmic measure of the mean probability, is computed according to

$$H(X) = -\sum p_i \ln(p_i)$$ (9.4)
It should be noted that for $p_i = 1$, $H(X) = 0$. Conversely, the entropy is a maximum value, $\ln(n)$, when $p_1 = \cdots = p_n = \frac{1}{n}$.

It has been shown in earlier work that the microstructure of a weld metal can be taken as having three principal constituents: acicular, allotriomorphic, and Widmanstätten ferrite (Bhadeshia et al., 1985; Abson and Pargeter, 1986; see also Chapter 5). It is important to emphasize that although $\alpha_a$ and $\alpha_w$ have similar strengths (Sugden and Bhadeshia, 1988), the weld metal microstructure cannot be treated as a two-phase microstructure (with $\alpha_a$ and $\alpha_w$ grouped together), since the toughnesses of the two phases are quite different. Therefore, the entropy of a given weld metal microstructure

$$H = -[V_a \ln(V_a) + V_a \ln(V_a) + V_w \ln(V_w)]$$

(9.5)

where $V_a$, $V_a$, and $V_w$ are the volume fractions of allotriomorphic, acicular, and Widmanstätten ferrite respectively.

The entropy of the distribution quantifies the heterogeneity of the microstructure. $H$ will vary from zero for an homogeneous material to $\ln 3$ (i.e. 1.099) for a weld with equal volume fractions of acicular, allotriomorphic and Widmanstätten ferrite. By multiplying by $(1/\ln 3)$, the heterogeneity of the three phase microstructure of a weld may be defined on a scale from zero to unity. i.e.

$$H_{et}^3 = H \times 0.910$$

(9.6)

A listout of the computer program used for the calculation of $H_{et}^3$ is included in Appendix 6.

As a secondary experiment, it was also decided to see if the primary and secondary regions of multipass welds could be treated similarly. Here, the secondary region is taken to comprise that part of the microstructure consisting of partially reaustenitised and significantly tempered regions (Svensson et al., 1988).

It follows that the heterogeneity of the assumed two-phase microstructure
\[
\text{Het}_2 = - [V_p \ln(V_p) + V_s \ln(V_s)] \times \left( \frac{1}{\ln 2} \right)
\]  

(9.7)

where \( V_p \) and \( V_s \) are the volume fractions of the primary and secondary regions respectively.

9.4 RESULTS

Initially, this work aimed to concentrate on analysing the primary (unrefined) regions of the weld metal. Data were taken from Watson et al. (1981) (Figure 9.3), and Bailey (1985) for two pass SA and triple arc SA welds respectively, and results for the estimation of scatter, and calculation of heterogeneity are given in Tables 9.1 and 9.2. Although Watson et al. (1981) referred to one of the phases observed as proeutectoid ferrite, this is a popular misnomer, and their description of this phase shows they meant allotriomorphic ferrite.

Figure 9.4 shows the relationship between the scatter observed in Charpy toughness values for the all-weld metal specimens and their microstructural heterogeneity.

Data for the calculation of \( \text{Het}_2 \) for the primary and reheated regions of multi-pass MMA low-alloy steel weld metals were taken from Abson (1982), and Taylor (1982). The work due to Taylor (1982) was particularly convenient since the Charpy data had been published numerically, rather than on a graph, and this facilitated the analysis. The percentage primary microstructure for Taylor’s welds, which were in accordance with ISO-2560, could be estimated from a knowledge of the compositions and the heat inputs of the welds (Svensson et al., 1988). It should be noted that the Charpy curves for W15SS and W15R (Abson, 1982) could not be included in this analysis, because the upper shelf energies for these welds were unevaluated. The various steps involved in the calculation of the scale parameter, and \( \text{Het}_2 \) for these data are summarised in Tables 9.3 and 9.4.

Figure 9.5 shows calculated values for the scatter obtained in Charpy toughness experiments on multirun weld metal specimens, as a function of microstructural heterogeneity, treating the weld as a two-phase microstructure.
<table>
<thead>
<tr>
<th>Weld</th>
<th>Reference</th>
<th>$E_{US}$/J</th>
<th>Deviance</th>
<th>$\nu$</th>
<th>Scale Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>AWO</td>
<td>Watson et al., 1981</td>
<td>183</td>
<td>6.54</td>
<td>13</td>
<td>0.503</td>
</tr>
<tr>
<td>FWO</td>
<td>&quot;</td>
<td>122</td>
<td>2.29</td>
<td>12</td>
<td>0.191</td>
</tr>
<tr>
<td>AW5</td>
<td>&quot;</td>
<td>134</td>
<td>6.96</td>
<td>11</td>
<td>0.632</td>
</tr>
<tr>
<td>FW5</td>
<td>&quot;</td>
<td>94</td>
<td>5.34</td>
<td>11</td>
<td>0.485</td>
</tr>
<tr>
<td>W1</td>
<td>Bailey, 1985</td>
<td>107</td>
<td>6.65</td>
<td>10</td>
<td>0.665</td>
</tr>
<tr>
<td>W2</td>
<td>&quot;</td>
<td>139</td>
<td>4.63</td>
<td>10</td>
<td>0.463</td>
</tr>
<tr>
<td>W4</td>
<td>&quot;</td>
<td>123</td>
<td>1.89</td>
<td>10</td>
<td>0.189</td>
</tr>
</tbody>
</table>

Table 9.1: Estimation of scatter for all-weld metal specimens.

<table>
<thead>
<tr>
<th>Weld</th>
<th>$V_\alpha$</th>
<th>$V_a$</th>
<th>$V_w$</th>
<th>$H$</th>
<th>Het$_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>AWO</td>
<td>0.29</td>
<td>0.67</td>
<td>0.04</td>
<td>0.756</td>
<td>0.688</td>
</tr>
<tr>
<td>FWO</td>
<td>0.09</td>
<td>0.89</td>
<td>0.02</td>
<td>0.380</td>
<td>0.346</td>
</tr>
<tr>
<td>AW5</td>
<td>0.50</td>
<td>0.47</td>
<td>0.03</td>
<td>0.788</td>
<td>0.717</td>
</tr>
<tr>
<td>FW5</td>
<td>0.25</td>
<td>0.08</td>
<td>0.68</td>
<td>0.817</td>
<td>0.744</td>
</tr>
<tr>
<td>W1</td>
<td>0.20</td>
<td>0.54</td>
<td>0.26</td>
<td>1.005</td>
<td>0.915</td>
</tr>
<tr>
<td>W2</td>
<td>0.18</td>
<td>0.69</td>
<td>0.13</td>
<td>0.830</td>
<td>0.755</td>
</tr>
<tr>
<td>W4</td>
<td>0.13</td>
<td>0.86</td>
<td>0.01</td>
<td>0.441</td>
<td>0.401</td>
</tr>
</tbody>
</table>

Table 9.2: Calculation of heterogeneity for all-weld metal specimens.
Figure 9.4: Showing the relationship between microstructural heterogeneity and scatter, as measured by the scale parameter of calculated Charpy curves. Each point corresponds to a complete set of Charpy results. The correlation coefficient is 0.94.
<table>
<thead>
<tr>
<th>Weld</th>
<th>Reference</th>
<th>$E_{US}/J$</th>
<th>Deviance</th>
<th>$\nu$</th>
<th>Scale Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>W18SS</td>
<td>Abson, 1982</td>
<td>184</td>
<td>1.10</td>
<td>8</td>
<td>0.138</td>
</tr>
<tr>
<td>W18R</td>
<td>&quot;</td>
<td>181</td>
<td>2.07</td>
<td>8</td>
<td>0.259</td>
</tr>
<tr>
<td>W19SS</td>
<td>&quot;</td>
<td>196</td>
<td>1.43</td>
<td>8</td>
<td>0.178</td>
</tr>
<tr>
<td>W20SS</td>
<td>&quot;</td>
<td>200</td>
<td>3.41</td>
<td>8</td>
<td>0.426</td>
</tr>
<tr>
<td>W20R</td>
<td>&quot;</td>
<td>199</td>
<td>2.86</td>
<td>8</td>
<td>0.358</td>
</tr>
<tr>
<td>W22R</td>
<td>&quot;</td>
<td>197</td>
<td>4.60</td>
<td>8</td>
<td>0.575</td>
</tr>
<tr>
<td>E7016</td>
<td>Taylor, 1982</td>
<td>205</td>
<td>16.6</td>
<td>18</td>
<td>0.922</td>
</tr>
<tr>
<td>E7016-1</td>
<td>&quot;</td>
<td>221</td>
<td>18.2</td>
<td>15</td>
<td>1.212</td>
</tr>
<tr>
<td>E7016-2</td>
<td>&quot;</td>
<td>195</td>
<td>27.1</td>
<td>18</td>
<td>1.503</td>
</tr>
<tr>
<td>E7016-3</td>
<td>&quot;</td>
<td>192</td>
<td>10.5</td>
<td>18</td>
<td>0.582</td>
</tr>
</tbody>
</table>

Table 9.3: Estimation of scatter for multirun welds.

<table>
<thead>
<tr>
<th>Weld</th>
<th>$V_p$</th>
<th>$V_s$</th>
<th>$H$</th>
<th>$Het_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>W18SS</td>
<td>0.38</td>
<td>0.62</td>
<td>0.664</td>
<td>0.958</td>
</tr>
<tr>
<td>W18R</td>
<td>0.32</td>
<td>0.68</td>
<td>0.627</td>
<td>0.905</td>
</tr>
<tr>
<td>W19SS</td>
<td>0.33</td>
<td>0.67</td>
<td>0.634</td>
<td>0.915</td>
</tr>
<tr>
<td>W20SS</td>
<td>0.35</td>
<td>0.65</td>
<td>0.647</td>
<td>0.934</td>
</tr>
<tr>
<td>W20R</td>
<td>0.43</td>
<td>0.57</td>
<td>0.683</td>
<td>0.985</td>
</tr>
<tr>
<td>W22R</td>
<td>0.24</td>
<td>0.76</td>
<td>0.551</td>
<td>0.795</td>
</tr>
<tr>
<td>E7016</td>
<td>0.30</td>
<td>0.70</td>
<td>0.611</td>
<td>0.881</td>
</tr>
<tr>
<td>E7016-1</td>
<td>0.37</td>
<td>0.67</td>
<td>0.636</td>
<td>0.918</td>
</tr>
<tr>
<td>E7016-3</td>
<td>0.42</td>
<td>0.58</td>
<td>0.680</td>
<td>0.981</td>
</tr>
<tr>
<td>E7016-3</td>
<td>0.48</td>
<td>0.52</td>
<td>0.692</td>
<td>0.999</td>
</tr>
</tbody>
</table>

Table 9.4: Calculation of heterogeneity for multirun welds.
Figure 9.5: Microstructural heterogeneity versus scatter for the MMA multipass welds analysed.
9.5 DISCUSSION

It can be seen from Figure 9.4 that there is a strong relationship between the scale parameter, and microstructural heterogeneity for low-alloy steel all-weld metals. This work implies that a significant part of the observed scatter in weld metal Charpy results is attributable to the inhomogeneity of the microstructure, with larger scatters being associated with more heterogeneous microstructures. This result can be compared with the fracture toughness experiments of Thaulow et al., (1987) who, for similar reasons, postulated that the most important factor in the COD testing of weldments is the positioning of the fatigue precrack.

The poor correlation for the multipass welds (Figure 9.5) highlights a limitation of this technique. Although, good results were obtained when the as-deposited microstructure was considered, the calculation of the heterogeneity of the microstructure of a given set of multipass welds must be carried out with caution. This is because the toughnesses of the two regions cannot be taken as independent. As was seen earlier (Figure 6.8), the strength of the secondary region is heavily dependent upon that of the primary from which it was formed. Of equal importance is the fact that the difference in the strengths of the as-deposited and reheated regions will depend upon alloy content, and will vary between steels, and it will therefore be necessary to take account of this in future work. Finally, Abson’s welds had a comparatively small number of readings per Charpy curve, and this might have introduced a further discrepancy into the equation.

9.6 THE EFFECT OF TEMPERING ON WELD METAL HARDNESS

In order to model the mechanical properties of multirun welds, it will be necessary to understand more fully the nature of the mechanical inhomogeneities in the microstructure, for which observable differences in microstructure are only a guide. For example, in multipass arc welds, the superheated zone in which the metal is reheated to just below its melting point is believed to be potentially very weak, giving lower Charpy and CTOD values than would otherwise be expected (Gretoft and Svensson, 1986). Similarly, it has also been suggested (Svensson, 1986) that the double-renormalised region in multirun weld deposits is potentially a very weak region. A possible reason for this could be strain ageing. For example, strain ageing is believed to cause localised hardness in weld deposits, making root regions of MMA weld deposits harder and stronger than subsurface regions (Abson, 1982). If
strain ageing were to be found to cause a small region of high hardness in a weld, this would then be a potential source of weakness.

To illustrate this point, samples from the top beads of three ISO-2560 welds, used elsewhere within this dissertation (Welds 6.2, 6.3 and 10.1), and whose compositions are given in Table 9.5, were extracted.

<table>
<thead>
<tr>
<th>Weld Composition, wt%</th>
<th>ppm by wt.</th>
</tr>
</thead>
<tbody>
<tr>
<td>ID. C Mn Si P S Cr Ni Mo Ti Al N O</td>
<td></td>
</tr>
<tr>
<td>6.2 0.10 1.56 0.42 0.015 0.007 0.04 0.04 0.01 0.013 0.015 119 262</td>
<td></td>
</tr>
<tr>
<td>6.3 0.15 1.57 0.45 0.012 0.007 0.04 0.03 0.01 0.014 0.015 96 193</td>
<td></td>
</tr>
<tr>
<td>10.1 0.32 1.65 0.48 0.015 0.005 0.03 0.03 0.01 0.018 0.015 64 141</td>
<td></td>
</tr>
</tbody>
</table>

Table 9.5: Concentrations of alloying additions in Welds 6.2, 6.3, and 10.1.

The welds were then tempered at temperatures up to 600°C for one hour. The specimens were quenched upon removal from the furnace to obviate any diffusion during cooling. (It should be emphasized that quenching would not cause any change in microstructure, because tempering was carried out below the A<sub>e1</sub> temperature). Twenty hardness measurements (Vickers 10kg) were then made of the top bead of each of the weld metal specimens. The results obtained are summarised in Table 9.6, and plotted in Figure 9.6.

<table>
<thead>
<tr>
<th>1 hour at T°C</th>
<th>VHN(10)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Weld 6.2</td>
</tr>
<tr>
<td>21</td>
<td>232</td>
</tr>
<tr>
<td>290</td>
<td>277</td>
</tr>
<tr>
<td>420</td>
<td>271</td>
</tr>
<tr>
<td>502</td>
<td>238</td>
</tr>
<tr>
<td>605</td>
<td>239</td>
</tr>
</tbody>
</table>

Table 9.6: Hardness readings (VHN(10)) (with 95% confidence limits) for Weld 6.2, 6.3, and 7.1 after 1 hour at four different temperatures.

It can be seen that in all three cases, clear evidence of strain ageing, in terms of an increase in recorded Vickers hardness, has been obtained. The increases in hardness, as a result of the short tempering treatment, correlate with the nitrogen
Figure 9.6: The hardnesses of Welds 6.2, 6.3, and 10.1 (with 95% confidence limits) after tempering for one hour at a temperature T. (The thermocouple accuracy has been taken as ±10°C, although, in reality, this probably underestimates its accuracy).
contents of the three welds (see Table 9.5), and can be construed to be due to the migration of nitrogen atoms to dislocations in the weld metal (Honeycombe, 1981b). Thus, Weld 6.2 increased more in strength than Weld 6.3, and Weld 10.1 increased in strength only slightly. Whatever the mechanism, these results imply that the strength of those regions of a multirun weld metal immediately below the fusion boundary which experience an equivalent tempering treatment during welding (i.e. equivalent in terms of the combination of tempering temperature and time) will be greater than that of the as-deposited weld metal. Thus, regions of local hardness will exist within the microstructure of multirun weld deposits where they will be liable to influence the fracture behaviour of that weld metal.

9.7 SUMMARY

A new method of interpreting weld metal toughness data characterised by wide scatter over a range of temperatures has been proposed. The microstructure of all-weld metal specimens has been treated as consisting of three independent phases: allotriomorphic ferrite, acicular ferrite, and Widmanstätten ferrite. Comparison with experimental data from the literature has shown that for all-weld metal specimens the scatter in weld metal toughness results can be related to the composition of the microstructure, and that the scatter observed is not wholly due to experimental error, but is a quantifiable function of the microstructure. For multirun weld metal specimens, however, agreement was poor. This can be attributed to two reasons. Firstly, that the model is only suitable when the toughnesses of the phases comprising the weld metal microstructure are non-interdependent, and secondly, as has also been shown, the microstructure of multirun welds will be likely to contain areas of localised hardness within regions of the same microstructure, and these will influence the toughness values recorded.

This work should permit the better design of experiments for the investigation of impact transition curves. It is also possible to estimate the error inherent in Charpy toughness results as a function of microstructure, and to plot a theoretical scatter band corresponding to scatter for mixed and homogeneous weld microstructures. This method could also be applied to aid the interpretation of weld metal COD results. Note, however, that at this stage the correlation between scatter and microstructure is empirical.
REFERENCES


MANDZIEJ, S. and SLEESWYK, A. W. (1987), "Welding Metallurgy of Struc-


10.1 INTRODUCTION

There is general agreement that a weld microstructure primarily containing acicular ferrite will exhibit high strength and excellent toughness due to its small grain size, high dislocation density, and the way in which the plates are dispersed in the microstructure (Pargeter, 1983; Sneider and Kerr, 1984). In contrast, the presence of allotriomorphic ferrite, ferrite plates with aligned carbides, or grain-boundary nucleated bainite is considered detrimental to the toughness of the weld, because these constituents allow cracks to propagate without much deflection. The problem is, in fact, more complicated, since it appears that a microstructure consisting totally of acicular ferrite does not exhibit optimum toughness, and that, ideally, a finite amount of allotriomorphic ferrite should also be present in the microstructure (Sneider and Kerr, 1984). Whatever the optimum microstructure, it is clear that a better understanding of the phases involved would permit more detailed investigation on the relationship with mechanical properties. In this context, acicular ferrite is the least understood of all the main phases that occur in steel welds. This work follows on from the work of Yang and Bhadeshia (1987), and Strangwood and Bhadeshia (1987), aimed at identifying and classifying acicular ferrite.

Over many years, the nature of the acicular ferrite phase has been the cause of much speculation. In point of fact, the term “acicular ferrite” is a misnomer. In two dimensions, acicular ferrite appears as randomly-oriented, needle-shaped particles (Figures 10.1a and b), but this belies its true morphology which is that of thin lenticular plates, typically 10μm long and apparently ~ 1μm wide (Bhadeshia, 1987). For a typical low-alloy C-Mn steel weldment, acicular ferrite will begin to appear during cooling in the range 500-440°C (Ito et al., 1982), and its exact nature has, until recently, been a matter for debate. Its ambiguous appearance has sometimes led workers to propose that it is Widmanstätten ferrite (Abson et al., 1978; Cochrane and Kirkwood, 1978). However, a series of experiments (Yang and Bhadeshia 1987; Strangwood and Bhadeshia, 1987), has now shown that acicular ferrite is essentially identical to bainite. It differs morphologically from bainite.
Figures 10.1a and b: Microstructure of acicular ferrite in (a) reaustenitised and isothermally transformed weld metal, and (b) low-C-Mn weld deposit. (After (a) J.-R. Yang (1987), and (b) M. Strangwood (1987), Ph.D. theses, University of Cambridge, U.K.).
found in wrought steels because it nucleates intragranularly on inclusions, and, in low-alloy steel weld deposits, is unable to adopt a sheaf morphology because of physical impingement with other plates nucleated nearby.

In order to put the work that follows in context, it is first instructive to discuss the bainite reaction in steels.

10.2 THE FORMATION OF BAINITE

Bainite forms by the decomposition of austenite at a temperature above the martensite start ($M_s$), but below that of fine pearlite. Microstructural and kinetic studies can become very complicated since, in low alloy steels, there is considerable overlap between the pearlitic and bainitic temperature ranges. In medium alloy steels, however, the two regions are more distinct, and give isothermal temperature-time-transformation (TTT) diagrams containing two separate C curves. The lower curve usually exhibits a flat top, and this corresponds to the bainite start ($B_s$) temperature (Zener, 1946).

Bainite grows in the form of sheaves of lenticular platelets of ferrite separated by regions of austenite ($\gamma$), martensite ($a'$), or cementite ($\theta$). The ferrite plates have a thickness of about $0.5 - 0.7\mu m$ (Oblak and Hehemann, 1967), although this varies with transformation temperature and alloy composition. The transformation is accompanied by a shape change which is an invariant-plane strain (I. P. S.) (Speich, 1962), and the bainitic subunits have the same, or nearly the same, crystallographic orientation with respect to one another.

Bainite is found in two district morphologies: upper bainite and lower bainite. Upper bainite consists of platelets of ferrite which are adjacent to one another, and in very nearly the same orientation in space. The ferrite platelets have the same habit plane (Ohmori, 1971; Sandvik, 1982) and comprise a sheaf which has a thin wedge plate morphology in three dimensions (Bhadeshia and Edmonds, 1980), as shown in Figure 10.2. The sheaves nucleate at austenite grain boundaries and have a rational orientation relationship (i.e. Kurdjumov-Sachs and Nishiyama-Wasserman type) with the austenite. Since upper bainite forms at higher temperatures when the yield strength of austenite is relatively low, plastic relaxation of the shape change leads to a high dislocation density in the surrounding ferrite (Bhadeshia and Edmonds, 1979).
Lower bainite is distinguished from upper bainite by the presence of carbide precipitation within the constituent ferrite subunits. These carbides, when they are cementite, precipitate in a variant of the Pitsch orientation within a subunit (Shackleton and Kelly, 1967), frequently at about 60° to the subunit long direction, the single variant arising from the need to minimise strain energy (Bhadeshia, 1980). Thorough crystallographic analysis (Bhadeshia, 1980) has shown the absence of the expected three phase $\alpha - \gamma - \theta$ orientation relationship, indicating that the carbides do not form by interphase precipitation. They might, therefore, precipitate either from the austenite during transformation, or from supersaturated ferrite. The low solubility of carbon in ferrite relative to austenite suggests intuitively the latter mechanism, and becomes an unavoidable conclusion of the discussion below.

A noteworthy feature of the bainite transformation is the phenomenon of incomplete reaction (Bhadeshia and Edmonds, 1980; Christian and Edmonds, 1984) in which, provided no interfering secondary reactions occur, transformation within the bainite range is found to produce only a limited amount of bainitic ferrite, the maximum extent of transformation increasing from zero with undercooling below the $B_s$ temperature. Cessation of the reaction occurs before the carbon content of the remaining austenite reaches the equilibrium value calculated by extrapolating the $Ae_3$ curve. This incomplete reaction phenomenon can be understood thermodynamically (Bhadeshia and Edmonds, 1980). The reaction stops when it is thermodynamically impossible to obtain composition invariant transformation. This condition is described by the $T_o$ curve on the phase diagram, which defines the locus of all temperatures where austenite and ferrite of the same composition have the same free energy. For the bainite reaction, the matrix will tend to physically restrain the shape change due to transformation from austenite, and this gives rise to a strain and surface energy of approximately 400 J/mol. Consequently a new $T_o$ curve, $T_o'$, may be defined to include the effects of this stored energy of 400 J/mol. This curve is at slightly lower carbon concentrations than the $T_o$ curve, and any displacive diffusionless transformation must occur below it. In a similarly way, a no-substitutional partitioning ($Ae_3'$) curve, for which transformation occurs without the redistribution of substitutional alloying elements, can be defined. Figure 10.2 shows dilatometric results obtained in low alloy C-Si steels in which cementite formation is inhibited allowing the true final content of the carbon in the austenite to be measured. Both the upper and lower bainite reaction were observed to terminate when the residual austenite composition reached the $T_o'$ curve. The ex-
Figure 10.3: Thermodynamic analysis of the bainite transformation. The \( \text{Ae}_3' \) line indicates the position of the no-substitutional partitioning (paraequilibrium) curve. Dilatometric analysis (○) shows the austenite carbon content at the termination of the bainite reaction to be in good agreement with the \( \text{T}_0' \) curve. (After H. K. D. H. Bhadeshia and D. V. Edmonds (1980), *Acta Metall.*, 28, 1265-1273).
planation for the incomplete reaction phenomenon, therefore, is that the bainitic ferrite forms with a supersaturation of carbon, which subsequently diffuses into the surrounding austenite. This means that the next subunit to form will do so from austenite which is enriched with carbon, and so under a reduced driving force. Bainite formation stops when sufficient carbon has diffused into the austenite that the b.c.c. and f.c.c. structures of the same composition have the same free energy. The fact that for some of the points in Figure 10.3 the amount of transformation exceeds that theoretically predicted can, in part, be attributed to later evidence (Bhadeshia and Waugh, 1982) that an inhomogeneous distribution of carbon exists during transformation, leading to a greater amount of reaction than that calculated on the basis of the average carbon content of the residual austenite. Reynolds et al. (1984) interpret these results qualitatively in terms of a solute drag effect at the \( \alpha/\gamma \) interface. However, their mechanism is not clearly explained, and much other research relating to the formation of bainite is also incompatible with a diffusional, and strongly supportive of a displacive transformation mechanism. This includes the following observations:

- Prolonged holding at the bainite reaction temperature has been observed to yield pearlite after the bainite reaction (Bhadeshia and Edmonds, 1979).

- The growth rate of bainite, monitored in situ using photo-emission electron microscopy (Bhadeshia, 1984) has been observed to be many orders of magnitude higher than that expected from carbon-controlled growth.

- Field ion microscopy (Bhadeshia and Waugh, 1982) has shown there to be a uniform distribution of substitutional alloying elements at the transformation interface. The complete absence of substitutional solute segregation mean that solute drag models are not tenable.

In summary, therefore, the bainite transformation seems to be described best by a displacive transformation mechanism. The bainite subunits form in an initial f.c.c.\( \rightarrow \)b.c.c. transformation involving an I. P. S. shape change. This gives rise to surface relief and a characteristic habit plane and orientation relationship. At this stage the bainitic ferrite has a composition identical to that of the surrounding austenite. Subsequently, the regions of residual austenite between the platelets of ferrite decompose either diffusonally to cementite (or other carbides) and ferrite, or partially decompose to martensite during cooling to ambient temperature with
carbon partitioning into the residual austenite. For lower bainite, which forms at lower temperatures than upper bainite, the process of partitioning of carbon into the residual austenite is expected to be slower, and hence some of the excess carbon precipitates within the bainitic ferrite. \(\varepsilon\)-carbide or \(\theta\) precipitates form to relieve the carbon supersaturation within the bainitic ferrite. After nucleation at an austenite grain boundary, new platelets form autocatalytically on the pre-existing platelets to give the aggregation of platelets that comprise the classical bainite sheaves (Bhadeshia, 1987).

10.3 ACICULAR FERRITE

Acicular ferrite exhibits an incomplete reaction phenomenon during transformation, with the amount of reaction tending to zero as the temperature is raised towards the \(B_n\) temperature (Yang and Bhadeshia, 1987). The lenticular plates of acicular ferrite \(\left(\alpha_a\right)\) form by the same displacive mechanism as bainite, with the carbon redistributing into the austenite subsequent to the transformation. However, they adopt a different morphology because nucleation occurs intragranularly at inclusions within the grains, and also because sheaf growth is restricted by hard impingement with plates nucleated at adjacent sites.

The purpose of the present work was to confirm further the mechanism of acicular ferrite growth. There are no carbide particles found within acicular ferrite in steel weld deposits, so that it is better described as upper bainite. However, if the carbon concentration of the weld is increased (with an associated decrease in transformation temperature), then it should, by analogy with the bainite transformation in wrought steels, be possible to observe "lower acicular ferrite", which is identical to upper acicular ferrite except that it is expected to contain a particular kind of cementite precipitation with the ferrite.

10.4 EXPERIMENTAL METHOD

In order to be able to expect to see intragranularly-nucleated lower bainite, an unusual weld would have to be fabricated. Yang and Bhadeshia (1987) found that an acicular ferrite morphology was favoured when the grain size was large, and the inclusion content was high - both conditions likely to promote intragranular nucleation by providing a relatively high density of suitable heterogeneous nucle-
ation sites, and forestall impingement from grain boundary phases also forming as a consequence of austenite decomposition. Conversely, bainitic microstructures are found in welds when the alloy content is high, the oxygen content is low, and the austenite grain size is large. The first of these is expected to be the most powerful factor in influencing microstructure. However, unfortunately, highly-alloyed welds often give microstructures that are very difficult to interpret (Deb et al., 1987). Therefore a weld with a high (0.3 wt%) carbon content was chosen as the simplest way by which lower bainite could be expected to be seen. The concentration of the other alloying elements was kept deliberately low in order to facilitate microstructural interpretation.

Although a low weld metal oxygen context could lead to the generation of bainitic microstructures, by depriving the interior of the columnar grains of nucleation sites for acicular ferrite, this was not desired, since the experiment aimed to isolate intragranularly-nucleated, rather than grain-boundary nucleated, bainite. However, the oxygen content should not be high either, since multiple nucleation events would lead to hard impingement between plates, masking the morphology of the product phase. In light of this, an oxygen content in the range 100-200ppm seemed desirable.

An ISO-2560 multirun manual-metal-arc weld was fabricated from 200mm thick plate. The arc current and voltage were 180A and 23V respectively with DC positive electrode polarity and no preheat. The welding speed was approximately 4mm/s. In accordance with the specification, the maximum interpass temperature was 250°C. The carbon content of the weld metal was controlled using specially-designed 4mm diameter carbon-coated electrodes to give a weld metal whose composition is given in Table 10.1.

<table>
<thead>
<tr>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>Cr</th>
<th>Ni</th>
<th>Mo</th>
<th>P</th>
<th>S</th>
<th>O</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.32</td>
<td>0.48</td>
<td>1.65</td>
<td>0.03</td>
<td>0.03</td>
<td>0.01</td>
<td>0.011</td>
<td>0.005</td>
<td>0.0141</td>
<td>0.0064</td>
</tr>
</tbody>
</table>

Table 10.1: Weld 10.1: Weld metal composition analysis (wt%)

It can be seen that the oxygen content is within the range intended.

Electrolytic etching of the weld metal was carried out in an aqueous solution of 20% NaOH by volume, at a voltage of 10 volts, for 45 seconds. Thin foils for transmission electron microscopy were prepared from 3mm diameter discs machined
from the top (unreheated) bead of the weld. The discs were ground sequentially on 400, 1200 and 4000 mesh SiC paper to a thickness of 0.05mm, and then electro-chemically profiled using a twin-jet Fischione electropolisher. Polishing was carried out at a voltage of 40V and at room temperature, in an electrolyte of 5% perchloric acid/25% glycerol in ethanol.

10.5 RESULTS

Figure 10.4 shows the solidification microstructure of the top bead of the weld. As was discussed in Chapter 2, because of the high cooling rates found in MMA welding, a carbon content of 0.30 wt% or greater will be liable to induce solidification from the melt as austenite in a low-alloy steel, rather than δ-ferrite. That solidification occurred as austenite is confirmed by the strong directionality of the microstructure due to unrestricted grain growth in the liquid phase, and by the fact that the cells within the grains change orientation only at the columnar boundaries. Near the weld centreline, which was the region of the weld that solidified last, a transition from a cellular to cellular-dendritic morphology can be observed, resulting from a build-up of solute ahead of the solidifying interface.

Figure 10.5 shows details of the microstructure with the specimen etched in nital. The cell boundaries can be seen to delineated by a discontinuous phase. The interior of the cells is difficult to resolve. Hardness testing was used to help characterize the microstructure. The hardness of the specimen (Vickers 10kg) was found to be (with a 95% confidence) 299 ± 2.2HV. Using a Zeiss microhardness tester, the dark region of the weld metal structure (i.e. the microstructure within the cells) gave a hardness of 448 ± 32HV. However, microhardness measurements of the discontinuous grain boundary phase gave a reading of 664 ± 36HV. This indicates that although the cell boundary phase superficially resembles allotriomorphic ferrite, it is martensitic in nature. In fact, martensitic formation at cell boundaries can be seen in high strength weld deposits, due to the large amount of solute segregation that occurs during solidification (Grong and Matlock, 1986). However, this does not appear to have been seen previously in low C-Mn welds. The most likely reason is that low-alloy steels usually solidify as δ-ferrite when the resultant alloying element segregation is not great. In this work, however, solidification occurred as primary austenite, which characteristically results in a much larger amount of chemical microsegregation, making martensitic formation at the cell boundaries
Figure 10.4: Weld metal microstructure showing solidification structure. Lightly electrolytically etched in saturated aqueous sodium hydroxide, followed by 2% nital.

Figure 10.5: Microstructure of the as-deposited weld metal. Vickers (10 gram)hardnesses are indicated for cell boundaries, and for the weld metal microstructure between them. Etchant: 2% nital.
more likely.†

The weld proved difficult to etch, probably because of its unusual composition, and, as will be seen later, profuse cementite precipitation. However, the microstructure of the weld was successfully revealed by electrolytic etching in saturated aqueous sodium hydroxide (Figures 10.6a and b), and a dilute preparation of nital, when the weld was found to contain a large amount of fine-grained acicular ferrite. Inclusions can also be seen in Figure 10.6a located at the cell boundaries, thus confirming earlier work described in Chapter 3.

Transmission electron micrographs of the weld are given in Figures 10.7-10.14. The microstructure of the weld metal at the prior austenite grain boundaries consisted predominantly of grain boundary nucleated upper bainite, as shown in Figures 10.7a and b. The high alloy concentration and high amount of solute segregation associated with solidification as austenite meant that allotriomorphic ferrite formation was inhibited, and this led to a microstructure at the grain boundaries completely different to that normally encountered in low-carbon C-Mn weld deposits where allotriomorphic ferrite and Widmanstätten ferrite are the predominant phases.

Within the columnar grains, the usual platelets of acicular ferrite, which are

†It will be noted that the microhardness readings of the individual phases are both higher than that of the weld as a whole. This occurs are a consequence of the so-called “indentation size effect”. It is an observed phenomenon that hardness measurements obtained from a material increase with decreasing load (O’Neill, 1967; Sargent, 1986). Although this behaviour has been explained for single crystals (Upit and Varchenya, 1973), it is not fully understood why polycrystalline materials should behave in this manner. One reason may be that friction is playing a part. Alternatively, for large deformations, grains partly slip over one another, so that the resultant deformation area is increased slightly. Generally, this effect goes unnoticed. However, the microhardness measurements in this work had to be made using the smallest available load to ensure that the indent size was much less than the dimensions of the cell boundary phase. The applied load was, therefore, only 1/1000th the macroload of 10kg, and this caused the observed hardness to increase. However, the comparison made between the hardnesses of the two phases recorded for the same applied load is still quite valid.
Figures 10.6a and b: Weld 10.1: Details of the as-welded microstructure. (a) electrolytically etched in saturated aqueous sodium hydroxide, and (b) etched in 0.5% nital.
Figures 10.7a and b: Classical bainite subunits nucleated at the prior austenite grain boundaries of Weld 10.1. The grey phase between the subunits in Figure 7a is likely to be retained austenite. Lower bainitic carbides (arrowed) may be seen within the ferrite, towards the top right of Figure 7b.
an instantly recognizable feature of low-carbon weld deposits were present, corresponding to intragranularly-nucleated bainite (Figure 10.8a). Other bainitic subunits appear to have nucleated around these laths in the same way that the formation of acicular ferrite in low-carbon C-Mn weld deposits is characterised by the sympathetic nucleation of $\alpha_a$ on pre-existing laths. Further evidence of the bainitic nature of the microstructure is given in Figure 10.8b.

In addition to the conventional acicular ferrite platelets, spectacular formations of intragranularly-nucleated “lower acicular ferrite” plates were also observed (Fig. 10.9). These were in all respects identical to conventional acicular ferrite, except that each plate contained a single orientation variant of cementite precipitates inclined to the plate axis. The cementite particles exhibited a Bagaryatski orientation relationship with the ferrite in which they precipitated. The microstructure of the lower acicular ferrite plates was found to be exactly identical to that of lower bainite in wrought steels, except that the clusters of plates nucleated at inclusions are not in the form of sheaves. The fact that a mixed microstructure of carbide-free acicular ferrite (i.e. intragranularly-nucleated upper bainite), and lower acicular ferrite (i.e. intragranularly-nucleated lower bainite) was observed, is probably a reflection of the fact that the microstructure formed by continuous cooling transformation.

Figures 10.10 and 10.11a and b show another region from the weld metal, emphasizing the large amount of cementite precipitation that has taken place within the bainitic ferrite. Figure 10.12a shows a high magnification micrograph of the the lower bainitic microstructure, comprising carbides within heavily dislocated ferrite. Figure 10.12b demonstrates that the carbides exhibit a Bagarystskii orientation relationship with the ferrite. Of all the phases that may form during the cooling of austenite, this orientation relationship is specific to lower bainite, and so proves the identity of the phase. Further details of the as-welded microstructure are shown in Figures 10.13 and 10.14.

10.6 DISCUSSION

The growth of lower bainite in a weld in the manner of intragranularly-nucleated plates has been hitherto unseen. The development of this highly unusual microstructure may be interpreted as being a consequence of the relatively high amount of carbon present in the weld, for, in general, a high carbon concentration will lead to an increased likelihood of bainite formation. Figure 10.15 shows a
Figures 10.8a and b: Microstructure of weld metal within the columnar grains, showing (a) long parallel subunits, comprising bainitic sheaf (arrowed), apparently nucleated on inclusion, and (b) higher magnification micrograph of bainitic sheaves.
Figure 10.9: Weld metal microstructure showing lower acicular ferrite.
Figure 10.10: Photo-montage of the microstructure of Weld 10.1 within the columnar grains showing classical lower bainitic microstructure.
Figures 10.11a and b: (a) Bright field image of weld metal microstructure, and (b) diffraction pattern taken from (013) cementite spot.
Figures 10.12a-c: (a) High magnification micrograph showing carbides within ferrite matrix, (b) diffraction pattern, and (c) interpretation of diffraction pattern. The carbides exhibit a Bagaryatski orientation relationship with the ferrite matrix.
Figures 10.13a-c: (a) Micrograph of bainitic subunits with carbides within them, (b) diffraction pattern, and (c) interpretation of diffraction pattern, showing two adjacent ferrite plates have an [011]∥[113] orientation relationship.
Figure 10.14: Micrograph quintessentialising the microstructure of Weld 10.1. The micrograph shows a spherical oxide inclusion surrounded by bainitic ferrite. Sub-units of upper and lower bainite may both be seen. Note the high dislocation density within the upper bainite.
Figure 10.15: Isothermal time-temperature-transformation diagrams for a steel with the same composition as Weld 10.1, and for compositionally equivalent steels with 0.08 and 0.16 wt% C. Calculated after the method due to Bhadeshia (1982).
calculated isothermal time-temperature-transformation (TTT) diagram for a steel with the same composition as Weld 10.1, and compares this with TTT curves calculated for steels with one half and one quarter the carbon concentration of the weld metal. [The curves are calculated using a program due to Bhadeshia (1982), which is based on a modification of Russell’s nucleation work (1968; 1969)]. Although Figure 10.13 should only be interpreted qualitatively, since, in reality, weld deposits are chemically inhomogeneous, and austenite decomposition occurs by continuous cooling, nevertheless, the retardation of the pearlite start temperature, and increased prominence of the bainitic region for increasing carbon concentrations can clearly be seen, showing that bainite formation in Weld 10.1 is possible, and not unexpected.

Since it is necessary to distinguish between the two bainitic phases observed, it is, therefore, proposed that they should be referred to as upper acicular ferrite, and lower acicular ferrite. Upper acicular ferrite is identical to the acicular ferrite habitually found in low-carbon weld deposits. Lower acicular ferrite has not been seen before, and corresponds to ferrite that has nucleated on inclusions, or sympathetically on laths of either upper or lower acicular ferrite, during continuous cooling of the weld. It is the phase that would be seen if the weld were to be reaustenitised, and isothermally transformed in the lower bainitic region.

10.7 SUMMARY

The microstructure of an ISO-2560 geometry 0.32C-1.65Mn-0.48Si (wt%) manual-metal-arc weld has been examined optically, and in the transmission electron microscope. The as-welded structure was found to consist of straight prior austenite grains which has solidified as the primary phase. Microhardness measurements demonstrated that the cell boundaries of the weld metal microstructure were largely martensitic, the martensite forming as a consequence of the relatively large amount of chemical segregation that results from austenitic solidification.

Transmission electron microscopy revealed that the microstructure of the weld was predominantly bainitic. Upper bainite was found nucleated at the grain boundaries, and as sheaves within the columnar grains. In the latter case, nucleation appeared to have occurred initially on inclusions. A large part of the microstructure consisted of lower bainite, which is a phase that is completely uncharacteristic of low-carbon weld deposits. The lower bainite formed due to the increasing difficulty
of carbon diffusion, and the carbon enrichment of the austenite, that occurred as the weld cooled. The likelihood that lower bainite will nucleate intragranularly on inclusions to form acicular ferrite in the same manner as upper bainite has led to the submission of a new nomenclature. It is suggested that upper bainitic acicular ferrite, which is the acicular ferrite phase habitually found in low-alloy steel weld deposits, be referred to as upper acicular ferrite when necessary to contrast it with acicular ferrite which formed as lower bainite. The latter should more precisely be referred to as lower acicular ferrite.
REFERENCES


CHAPTER 11

A PROGRAMME FOR FUTURE RESEARCH

This work tackled a broad range of issues. Throughout this project, however, the central aim has been to further our ability to quantitatively predict weld metal properties.

The discovery that the inclusions in weld deposits are not uniformly distributed is an important step towards being able to model the inclusion distribution in steel weld deposits. The precise mechanism, and the factors which influence this behaviour could be found using transparent organic media, seeded with inert powders to act as inclusions. In this way, the process of inclusion redistribution could be observed as it occurred, during solidification. Similarly, the effect of inclusion size distribution could also be investigated using low melting point alloys with carefully-characterised particle sizes. With a knowledge of the initial size distribution of the inclusions in the melt, and the dimensions of the primary columnar grains, the final distribution of these inclusions could be estimated. The quantity of secondary indigenous inclusions in the weld is also calculable. Their formation is a consequence of solute accumulation at the grain boundaries, and will be largely dependent upon alloy composition and the cooling rate of the melt. Together these give an overall picture of the total distribution of inclusions in the weld deposit from which many important parameters, such as the spacing, distribution and size distribution of the inclusion may be determined.

Detailed analysis of the inclusion distributions of a wide variety of welds is required, so that those factors that determine their ultimate volume fraction, size distribution, and mean particle size can be understood, since these are now recognized to be so important in controlling the strength and toughness of the weld. As precise information is the dispersion characteristics is needed, this investigation could probably best be done using carbon replica techniques in the transmission electron microscope. The experimental procedures involved are well-documented (A. S. T. M., 1973), and their usefulness in weld metal analysis is being recognized (Pacey et al., 1982; Keville, 1983; Liu, 1987). The deposition of an amorphous layer of carbon allows the study of large specimen areas. Also, microanalysis of individual inclusions is facilitated since the matrix is absent, although an image
of the microstructure is retained on the replica. Finally, replicas guarantee the extraction of large inclusions, which can fall out of foils.

It has been shown (Gretoft et al., 1986) that, on a microscopic scale, the concentration of alloying elements in a weld is not constant. It would, therefore, be of particular interest to see how fluctuations in the local concentration of alloying elements in a given weld deposit can be related to its microstructure. This research would involve obtaining detailed composition profiles across the cell and columnar grain boundaries of a weld, and, on a larger scale, from the fusion boundary to the centre of the weld, since centreline segregation would tend to cause solute to accumulate ahead of the solidifying interface to give a slightly higher substitutional alloying element concentration in the centre (Davies and Garland, 1975). The influence of chemical segregation in relation to the position of the inclusions also merits investigation, but has yet to be studied.

A systematic study is required of the solidification behaviour of steel welds so that the identity of the solidifying phase can be predicted for a given alloy as a function of cooling rate. The general characteristics of weld metal solidification need to be established. For example, it would be interesting to see if the cooling curves for ferritic and austenitic solidification are visibly different in terms of the rate at which heat is removed from the weld. These results would then be combined with diffusion theory to allow the calculation of the growth rates of δ and γ dendrites as a function of alloy composition. Combined with the thermodynamic work described in this dissertation, the results would be represented in the form of isothermal solidification (solid/liquid) temperature-time-transformation curves. The appearance of the curves would alter depending upon what nuclei were present. For example, in a low carbon weld, nuclei of δ are present, and solidification as austenite is correspondingly difficult. If nuclei of austenite are present, however, then an austenitic solidification mode is likely to predominate.

A particularly interesting experiment in this line of research might be to weld a low-carbon electrode onto a high carbon steel plate, connected to a low carbon base plate. As with Weld 3.1, on the high carbon base plate, the weld metal would solidify as austenite. In such circumstances, it is possible that the austenitic mode of solidification would survive the transition across to the low-carbon base plate to give a weld solidification structure consisting of primary austenite grains on a δ-ferrite base plate. The details of such a structure would be of great general interest.
Practical measurement of the partitioning that occurs in the microstructure during solidification, perhaps by quenching in of weld deposits during welding would also be of interest.

The model for the strength of weld metals originated in this thesis should be developed in two ways. First, research must be undertaken to quantify how the microstructural strengthening contribution alters with temperature so that the variation of weld metal strength with temperature can be calculated. This could be done by measuring the strengths of a set of welds with carefully characterised microstructures. Ideally, testing should be carried out not only over a wide temperature range, but at a variety of strain rates, since testing at higher strain rates is equivalent to testing at lower temperatures. An ability to predict how yield strength varies with temperature has many potential applications; one example would be in the analysis of thermal stresses in welds. Large local stresses are known to exist in weld metals around inclusions due to differences in the coefficients of thermal contraction, and the elastic moduli of the inclusion and the matrix (Farrar and Harrison, 1987). However, the lack of directionality in the distribution of acicular ferrite, despite the strong temperature gradients, implies that thermal stresses are not a major factor in influencing inclusion nucleation.

Secondly, a series of systematic experiments to model the reheated regions of multirun weld deposits is needed, so that the microstructural changes that occur in the fusion zone during multilayer deposition can be analysed. A good way to do this would be to anneal a set of welds for increasing times in the temperature range of, say, 150-1000°C, and record how simple mechanical properties of the weld metals (e.g. hardness) vary with heat treatment. For temperatures above the eutectoid temperature, the effect of different cooling rates should also be measured, since these will affect the development of the reheated microstructure. (Such experiments might readily be carried out in a dilatometer, wherein cooling rates can be controlled very accurately). This work would provide data on how the microstructure of a weld changes for a given initial microstructure, heat treatment, and cooling rate, and, in this way, a detailed model could be constructed which would allow the strength of multirun welds to be predicted.

The upper shelf energy can sometimes be correlated with weld metal oxygen content (Devillers et al., 1984). However, this is only an indirect measure of the inclusion content, more precise details of which will have to be taken into account.
Many excellent data are available in the literature (Kayali et al., 1984; Bellrose, 1985; Thewlis, 1986) giving data for the Charpy toughness of welds together with detailed analyses of inclusion populations. Although, recent work has shown there to be a relationship between upper shelf energy and the ratio between the mean size of inclusions, and their mean spacing (Roberts et al., 1982), a widely-applicable satisfactory model has yet to be produced. The actual advance of a crack tip in a matrix with a given inclusion distribution should be modelled using finite element analysis.

Particular notice should also be taken of the effect of nickel additions on impact toughness. Nickel is known to have a beneficial effect on weld metal toughness (Pokhodnya et al., 1986), and this might be due to the softening effect which nickel was observed to noted in Chapter 6.

Also, since it is now possible to predict the flow stress and tensile strength of a weld as a function of temperature, an exciting advance from this would be to combine this work with established fracture theory to produce a model which would allow the calculation of the toughness transition temperature of a weld. Although, because the critical temperature at which, on cooling, cleavage failure becomes dominant is a function of, inter alia, the grain size and inclusion population of the weld (Bowen et al., 1986), a more detailed model of the microstructure will be necessary, and stereological measurements of the grain structure of weld metal fracture specimens would also have to be made.

In the interest of applicability, the work on elongation and reduction in area should become more generalised. For example, the factors which control the strain-hardenability of a weld should be considered, since this affects percentage elongation. From a practical point of view, the work-hardening rate will vary with a variety of welding parameters, particularly preheat, since this will affect cooling rates and the degree to which stresses can be annealed out during cooling. A model which would allow reduction in area to be predicted from the chemical composition of the weld (wt% [O], [S], [Mn], &c.) rather than a measured inclusion volume fraction, should also be adopted. It would also be desireable to try to model ductility, terms of elongation and reduction in area, as a function of temperature.

The observed relationship between scatter in Chapy results and the uniformity of the microstructure is a particularly interesting finding, and the next step should
be the application of this model to the calculation of the heterogeneity of multirun welds, which could be done most simply by treating the as-weld and reheat regions as hard and soft phases in a two-phase microstructure. This model could then be refined if found to be too simplistic. However, an important step in the development of this model, should be to take account of the mechanical heterogeneity of the microstructure. This is because a multiphase microstructure with phases of roughly equivalent toughness would be expected intuitively to exhibit less scatter during impact testing than one containing phases with vastly different properties, although the calculated heterogeneities of the microstructures might still be the same.

Finally, the discovery that lower bainite can form in low-alloy steel weld deposits, and its possible nucleation in inclusions, is of enormous interest. The microstructure is so unusual that a comprehensive TEM investigation is called for.
REFERENCES


APPENDIX 1: AE3 PROGRAM
1 FTVSCLR PROGRAM=%H! DATA=.PDP:INPUT NAG
2 C
3 C PROGRAM FOR THE CALCULATION OF THE AE3 TEMPERATURE
4 C FOR LOW-ALLOY STEELS
6 C ELEMENTS MUST BE INSERTED IN THE DATASET IN THE ORDER:
7 C Mn Si Ni Cr Mo Cu V Nb W Co
8 C
9 IMPLICIT DOUBLE PRECISION (T)
10 DOUBLE PRECISION A(10),AC,AI(10),B(10,5),C,C6,CAF,CF,CLIQ,D(10,6)
11 DOUBLE PRECISION DAT(10),DELTAT,DTALPH,DTGAM,E(10,4),FEAF,G,GC,GI
12 DOUBLE PRECISION H,H1,P,Q,R,WTPC,X(10),XX(10),Z,Z6,Z61
13 DOUBLE PRECISION HK(13),HC(13)
14 COMMON /INTER/B
15 COMMON /DELTA2/E
16 COMMON /PARMS/G,R,TO,T,P,CF,Q,GC,GI,H1,H
17 INTEGER ANS,COUNT,COUNTA,DUMMY,FLAG 1,FLAG2,s43,S54,S91
18 COUNTA = 2
19 K = 2
20 MM = 2
21 NCAP7 = 13
22 IFAIL = 0
23 R = 1.985800
24 C cal/mol/K
25 DATA C, SUM, DELTAT/0.0D0, 0.0D0, 0.0D0/
26 DATA TEMP, TT, Z/0.0D0, 0.0D0, 0.0D0/
27 C
28 C SPLINE COEFFICIENTS FOR DELTAoHo
29 C INTERPOLATES DATA FROM KAUFMAN ET AL. (RANGE 0-1183K)
30 C
31 DATA HK(1),HK(2),HK(3),HK(4)/0.0D0,0.0D0,0.0D0,0.0D0/
32 * HK(5),HK(6),HK(7),HK(8),HK(9)/1.5D2,3.0D2,7.2D2,9.6D2,1.08D3/
33 * HK(10),HK(11),HK(12),HK(13)/1.183D3,1.183D3,1.183D3,1.183D3/
34 * HC(1),HC(2),HC(3),HC(4)/1.303D3,1.272D3,1.368D3,1.703D3/
35 * HC(5),HC(6),HC(7),HC(8)/1.552D3,1.281D3,3.359D2,2.344D2/
36 * HC(9),HC(10),HC(11),HC(12)/2.134D2,0.0D0,0.0D0,0.0D0/
37 * HC(13)/0.0D0/
38 *************************************************************
39 WRITE(6,101)
40 WRITE(6,51)
41 WRITE(6,301)
42 WRITE(6,51)
43 READ(5,*) (DAT(I),I=1,10)
44 IF (ADD(DAT).EQ.0.0D0) THEN
45 WRITE(6,159)
46 ELSE
47 WRITE(6,160)
48 IF (DAT(1).NE.0.0D0) WRITE(6,161)DAT(1)
49 IF (DAT(2).NE.0.0D0) WRITE(6,162)DAT(2)
50 IF (DAT(3).NE.0.0D0) WRITE(6,163)DAT(3)
51 IF (DAT(4).NE.0.0D0) WRITE(6,164)DAT(4)
52 IF (DAT(5).NE.0.0D0) WRITE(6,165)DAT(5)
53 IF (DAT(6).NE.0.0D0) WRITE(6,166)DAT(6)
54 IF (DAT(7).NE.0.0D0) WRITE(6,167)DAT(7)
55 IF (DAT(8).NE.0.0D0) WRITE(6,168)DAT(8)
56 IF (DAT(9).NE.0.0D0) WRITE(6,169)DAT(9)
57 IF (DAT(10).NE.0.0D0) WRITE(6,170)DAT(10)
58 ENDIF
59 101 FORMA T(IX)
60 301 FORMAT(' A e 3 P R O G R A
61 1 M')
62 159 FORMAT(' Pure iron')
63 160 FORMAT(' The steel contains:')
64 161 FORMAT(F5.2,' wt% manganese')
65 162 FORMAT(F5.2,' wt% silicon')
66 163 FORMAT(F5.2,' wt% nickel')
67 164 FORMAT(F5.2,' wt% chromium')
68 165 FORMAT(F5.2,' wt% molybdenum')
69 166 FORMAT(F5.2,' wt% copper')
70 167 FORMAT(F5.2,' wt% vanadium')
71 168 FORMAT(F5.2,' wt% niobium')
72 169 FORMAT(F5.2,' wt% tungsten')
73 170 FORMAT(F5.2,' wt% cobalt')
74 ******************************************************
75 DO 1 I =1,10
76 1 XX(I) = DAT(I)
77 C wt%
78 DUMMY = 0
79 2 C6 = 0.0D0
80 NUM = 0
81 COUNT = 0
82 FLAG2 = 1
83 DTGAM = 0.0D0
84 Z61 = 1.0D2
85
86 WRITE(6,52)
87 WRITE(6,57)
88 WRITE(6,55)
89 WRITE(6,57)
90 3 CONTINUE
91 DO 17 N = 1,51
92 IF (COUNT.EQ.-1 .OR. COUNT.EQ.12) GOTO 17
93 IF (K.EQ.5 .AND. NUM.EQ.3) GOTO 17
94 C = (N-1)*0.01D0
95 4 CONTINUE
96 5 WTPC = C + ADD(XX)
97 IF (WTPC.GT.5.0) THEN
98 WRITE(6,52)
99 WRITE(6,53)
100 88 WRITE(6,54)
101 GOTO 88
102 ENDIF
103 C
104 C CALCULATION OF MOLE FRACTIONS
105 C
106 FEAF = (1.0D2-WTPC)/5.58D1
107 CAF = C/1.2D1
108 DO 6 M = 1,10
109 6 X(M) = XX(M)/B(M,1)
110 TAF = FEAF + CAF + ADD(X)
111 CF = CAF/TAF
112 DO 7 M = 1,10
113 7 X(M) = X(M)/TAF
114 CALL TZERO (CF,TO)
115 T = TO
116 H1 = -1.5325D4
69
117 11 CONTINUE
118 CALL GALGA(G,GC,T)
119 G = -G
120 IF (T.GT.1.183D3) THEN
121 C
122 C VALID UP TO 1360K
123 C
124 H = 2.549D3 - 2.746D0*T + 6.503D-4*T*T
125 G = 2.476D3-5.03D0*T+3.363D-3*T*T-7.44D-7*T*T*T
126 ELSE
127 CALL E02BBF(NCAP7,HK,HC,T,H,IFAIL)
128 ENDIF
129 AC = DEXP(GC/(R*TO)+(8.91D3/T)*CF)
130
131 SUM = 0.0D0
132 DELTAT = 0.0D0
133 DO 14 M = 1,10
134 IF (X(M).EQ.0) THEN
135 A(M)=0.0D0
136 AI(M)=1.0D0
137 GOTO 14
138 ENDIF
139
140 P = B(M,4) + B(M,5)/T
141 Q = 0.0D0
142 IF (M.EQ.1) THEN
143 C
144 C DATA FROM GILMOUR ET AL., MET. TRANS., 1972
145 C
146 GI = 6.118*T - 7808.0
147 ELSE
148 GI = E(M,1)+(E(M,2)+E(M,3)*T+E(M,4)*DLOG(T))*T
149 ENDIF
150
151 C
152 C CALCULATION FOR SOLUTE PARTITION COEFFICIENTS
153 C
154 AI(M) = DEXP(GI/(R*TO)+P*CF)
156 CALL EQN(A(M),K,C,CLIQ)
157 SUM = SUM + X(M)*A(M)
158 14 CONTINUE
159 DELTAT = SUM*R*TO*TO
160 T = TO+DELTAT
161 Z = TT - T
162 Z = DABS(Z)
163 IF (Z.LT.0.5D0) GOTO 15
164 TT = T
165 IF (K.EQ.2) GOTO 11
166 15 CONTINUE
167
168 IF (COUNT.EQ.-1) THEN
169 IF (DUMMY.NE.0) TEMP = T
170 GOTO 17
171 ENDIF
172 IF (K.EQ.3 .AND. S93.NE.3) THEN
173 WRITE(6,51)
174 ELSE
175 IF (S91.EQ.3 .AND. N.EQ.1) GOTO 17
176 IF (NUM.EQ.1) THEN
177 IF (T.LT.TEMP) THEN
178 COUNT = -1
179 GOTO 17
180 ELSE
181 WRITE(6,51)
182 ENDIF
183 ELSE
184 WRITE(6,63)C,T-273,AC
185 DO 16 I = 1,10
186 IF (AI(I).EQ.1.0D0) GOTO 16
187 IF (I.LT.9) THEN
188 WRITE(6,65)I+1, AI(I)
189 ELSE
190 WRITE(6,66)I+1, AI(I)
191 ENDIF
192 16 CONTINUE
193 ENDIF
194 ENDIF
195
CONTINUE
STOP

51 FORMAT(1X,61(1H-))
52 FORMAT(1X)
53 FORMAT(' The sum of the alloy components should not exceed 5wt%.')
54 FORMAT(1X,80(1H ))
55 FORMAT(' WT%C T/degreesC Partition coefficients')
56 FORMAT(1X,80(1H ))
57 FORMAT(' +--------+-------+
1-+')
58 FORMAT(' ',F5.2,' ',F6.1,' A(c) :',F6.3)
59 FORMAT(' A(',I1,') :',F6.3)
60 FORMAT(' A(',I2,') :',F6.3)
61 END

DATA FOR ALLOYING ELEMENT INTERACTION PARAMETERS

COMMON /INTER/B

DATA((B(M,J),J=1,5),M=1,10)/
5.49D1,0.00D0,-5.06D3,0.00D0,-5.07D3,
2.81D1,-4.28D-1,1.87404,4.84D0,-7.37D3,
5.87D1,0.00D0,5.34D3,-2.20D7,7.63D3,
5.20D1,0.00D0,-9.53D2,2.44D1,-3.84D4,
9.59D1,0.00D0,-7.49D3,3.855D0,-1.787D4,
6.35D1,0.00D0,7.586D3,0.00D0,4.23D3,
5.09D1,0.00D0,-3.01D4,0.00D0,-2.466D4,
9.29D1,0.00D0,-4.661D4,0.00D0,-2.877D4,
1.838D2,0.00D0,-1.223D4,2.34D1,-3.6214D4,
5.89D1,0.00D0,3.55D3,0.00D0,2.83D3/
END

DATA FOR ALLOYING ELEMENT FREE ENERGY CHANGES (DELTA G(I))

DATA((B(M,J),J=1,5),M=1,10)/
COMMON /DELTA2/E
DOUBLE PRECISION E(10,4)
DATA((E(M,J),J=1,4),M=1,10)/
C-2.665D4,4.269D1,-1.7D-2,0.0D0,
C5.65D2,1.5D-1,0.0D0,0.0D0,
C-2.55D4,4.1183D1,-1.7D-1,0.0D0,
C-8.357D3,1.38D1,-5.1D-3,0.0D0,
C
C NIOBIUM RECALCULATED
REF: A.A.B.SUGDEN, C.P.G.S DISSERTATION, 1986
C
C5.139D3,-2.892D0,0.0D0,0.0D0,
C2.5D3,1.5D-1,0.0D0,0.0D0,
CO.0D0,0.0D0,0.0D0,0.0D0/
END

DOUBLE PRECISION FUNCTION ADD(Y)
DOUBLE PRECISION Y(10)
ADD = 0.0D0
DO 4 I = 1,10
ADD = ADD + Y(I)
RETURN
END

THIS SECTION CONTAINS 2 SUBROUTINES TO FIND
C To AND DELTAGo RESPECTIVELY
SUBROUTINE TZERO (X1,T1)
DATA PROVIDED BY BHADESHIA
C RANGE 200-900 CENTIGRADE
C
DOUBLE PRECISION X1,T1
IF (X1.GE.6.88D-2) GOTO 1

***************
273 IF (X1.LT.1.00E-3) THEN
274 T1 = 9.11502 - 2.12E4*X1 + 3.4506E1*X1*X1
275 ELSE
276 IF (X1.LT.3.135E-2) THEN
277 T1 = 9.05602 - 1.068E4*X1 + 2.811E3*X1*X1 - 3.913E3*(X1**3)
278 ELSE
279 IF (X1.LT.4.840E-2) THEN
280 T1 = 8.55802 - 4.694E3*X1 + 2.156E4*X1*X1
281 ELSE
282 IF (X1.LT.1.00E-3) THEN
283 T1 = 7.47502 - 1.449E3*X1 - 7.163E3*X1*X1
284 ENDIF
285 ENDIF
286 GOTO 2
287 1 CONTINUE
288 IF (X1.LT.9.330E-2) THEN
289 T1 = 6.15202 + 1.779E3*X1 - 2.677E4*X1*X1
290 ELSE
291 IF (X1.LT.1.526E-1) THEN
292 T1 = 5.16802 + 5.017E3*X1 - 6.693E4*X1*X1
293 T1 = T1 + 1.823E5*(X1**3)
294 ELSE
295 T1 = 6.92202 - 1.087E3*X1 - 6.696E4*X1*X1
296 ENDIF
297 ENDIF
298 2 CONTINUE
299 T1 = T1 + 273
300 RETURN
301 END
302
303 SUBROUTINE GALGA (G2,GC2,TI)
304 C
305 C DATA DUE TO KAUFMAN, CLOUGHERTY, AND WEISS
306 C (RANGE 0-1183K)
307 C
308 DOUBLE PRECISION G2,GC2,TI
309 IF (T2.LT.7.00E2) THEN
310 IF (T2.LT.3.00E2) THEN
311 G2 = 1.38E0*T2 - 1.499E3
312 ELSE
313 G2 = 1.65786D0*T2 - 1.581D3
314 ENDIF
315 ELSE
316 IF (T2.LT.9.4D2) THEN
317 G2 = 1.30089D0*T2 - 1.331D3
318 ELSE
319 G2 = - 8.89909D0 + 2.6557D-1*(T2-1.14D3)
320 G2 = G2 - 1.04923D-3*(T2-1.14D3)*(T2-1.14D3)
321 G2 = G2 + 2.70013D-6*((T2-1.14D3)**3)
322 G2 = G2 - 3.58434D-9*((T2-1.14D3)**4)
323 C
324 C CORRECTED DATA PROVIDED BY BHADRESHIA AND YANG
325 C
326 ENDIF
327 ENDIF
328 GC2 = 7.686D0*T2 - 1.532504
329 RETURN
330 END
331 ******************************************
332
333 SUBROUTINE EQN (F16,NO,CC,CQIL)
334 IMPLICIT DOUBLE PRECISION (F)
335 DOUBLE PRECISION G,R,TO,T,P,CF,Q,GC,GI,Hl,H
336 DOUBLE PRECISION CC,CQIL,EGll,ELll
337 COMMON /PARMS/G,R,TO,T,P,CF,Q,GC,GI,H1,H
338 C
339 C SET CARBON-CARBON INTERACTION PARAMETERS
340 C
341 EGll = 0.0D0
342 ELll = 8.91D3/T
343 C
344 C MAIN EQUATION
345 C
346 F1 = GI/(R*TO) + P*CF
347 F2 = GC/(R*TO)
348 F3 = 1 + Q*CF*DEXP(F2)
349 F4 = GC/(R*TO) + (ELll)*CF
350 F5 = 1 + EGll*CF*DEXP(F2)
351 F6 = DEXP(F1)/F3
352 F7 = DEXP(F4)/F5
353 F8 = 1+CF*(1-CF)*(P-Q*F6*F7)
354 F9 = G/(R*TO*TO)
355 F10 = CF*CF/2*((EL11)-(EG11*F7*F7))
356 F11 = DEXP(F4)*CF*H1/F5
357 F12 = (1-CF)*H
358 F13 = F9 - F10
359 F14 = F11+F12*DEXP(F13)
360 F15 = F8*DEXP(F13)
361 F16 = (F6-F15)/F14
362 RETURN
363 END
364 !
APPENDIX 2: DETERMINATION OF $\Delta T$

The chemical potentials in the two phases are equal. Therefore, e.g., for the austenite liquidus.

$$X_o \gamma_o = X_o L \gamma_o L \exp \left( \frac{\Delta^o G_o^{\gamma - L}}{RT} \right)$$

Therefore

$$\frac{\Delta^o G_o^{\gamma - L}}{RT} = \ln \left| \frac{X_o \gamma_o}{X_o L} \right| + \ln |\gamma_o| - \ln |\gamma_o L|$$

(1)

Similarly, for the $i^{th}$ component

$$X_i \gamma_i = X_i L \gamma_i L \exp \left( \frac{\Delta^o G_i^{\gamma - L}}{RT} \right)$$

Therefore

$$\frac{\Delta^o G_i^{\gamma - L}}{RT} = \ln \left| \frac{X_i \gamma_i}{X_i L} \right| + \ln |\gamma_i| - \ln |\gamma_i L|$$

The Wagner (Taylor) activity formulae for a ternary system, with the standard state defined at infinite dilution, may be written
\[ \ln \gamma_o = -\frac{1}{2} \sum_{i, k=1}^{n} \epsilon_{ik} X_i X_k \]

and \[ \ln \gamma_i = \sum_{k=2}^{n} \epsilon_{ik} X_k \]

For Fe \((n = 0)\)

\[ X_o^\gamma = 1 - X_1^\gamma - \sum_{2}^{n} X_i^\gamma \]

and \[ X_o^L = 1 - X_1^L - \sum_{2}^{n} X_i^L \]

Therefore, from Eqn. (1)

\[ \frac{\Delta^o G_o^\gamma \rightarrow L}{RT} = \ln \left| \frac{1 - X_1^\gamma - \sum_{2}^{n} X_i^\gamma}{1 - X_1^L - \sum_{2}^{n} X_i^L} \right| - \frac{\epsilon_{11}^{\gamma}}{2} (X_1^\gamma)^2 \]

\[ - X_1^\gamma \sum_{2}^{n} \epsilon_{1i}^\gamma X_i^\gamma + \frac{\epsilon_{11}^L}{2} (X_1^L)^2 + X_1^L \sum_{2}^{n} \epsilon_{1i}^L X_i^L \]  \(2\)

Similarly, for C \((n = 1)\)

\[ \frac{\Delta^o G_1^\gamma \rightarrow L}{RT} = \ln \left| \frac{X_1^\gamma}{X_1^L} \right| + \epsilon_{11}^L X_1^\gamma - \epsilon_{11}^L X_1^L \]  \(3\)
and for component $i$

$$\frac{\Delta^\circ G_i^\gamma - L}{RT} = \ln \frac{X_i^\gamma}{X_i^L} + \epsilon_i^\gamma X_i^\gamma - \epsilon_i^L X_i^L$$

Rearranging Eqn. (3) gives

$$X_i^\gamma \exp(\epsilon_i^\gamma X_i^\gamma) = X_i^L \exp \left[ \frac{\Delta^\circ G_i^\gamma - L}{RT} + \epsilon_i^L X_i^L \right]$$

(4)

Similarly, for component $i$

$$X_i^\gamma \exp(\epsilon_i^\gamma X_i^\gamma) = X_i^L \exp \left[ \frac{\Delta^\circ G_i^\gamma - L}{RT} + \epsilon_i^L X_i^L \right]$$

(5)

Now

$$\exp \left[ \frac{\Delta^\circ G(T)}{RT} \right] = \exp \left[ - \frac{\Delta^\circ S}{R} \right] \exp \left[ \frac{\Delta^\circ H}{RT} \right]$$

Let $T = T_o + \Delta T$. Then

$$\exp \left[ \frac{\Delta^\circ G(T)}{RT} \right] = \exp \left[ - \frac{\Delta^\circ S}{R} \right] \exp \left[ \frac{\Delta^\circ H}{T_o} \right] \exp \left[ - \frac{\Delta^\circ H}{T_o} \right] \exp \left[ \frac{\Delta^\circ H}{R(T_o + \Delta T)} \right]$$

$$= \exp \left[ \frac{\Delta^\circ G_o}{RT_o} \right] \exp \left[ \frac{\Delta^\circ H T_o - \Delta^\circ H(T_o + \Delta T)}{RT_o(T_o + \Delta T)} \right]$$

79
Likewise

\[ \exp \left[ \frac{\Delta^\circ G_1}{RT} \right] = \exp \left[ \frac{\Delta^\circ G_1}{RT_0} \right] \exp \left[ \frac{-\Delta^\circ H \Delta T}{RT_0(T_0 + \Delta T)} \right] \]

At \( T = T_0 \)

\[ \exp \left[ \frac{\Delta^\circ G_i}{RT} \right] = \exp \left[ \frac{\Delta^\circ G_i}{RT_0} \right] \]

Therefore from Eqn. (4)

\[
X_1^L \exp(\epsilon_{11}^X X_1^L) = X_1^L \exp \left[ \frac{\Delta^\circ G_1^{\gamma-L}}{RT} \right] \exp(\epsilon_{11}^L X_1^L)
= X_1^L \exp \left[ \frac{\Delta^\circ G_1}{RT_0} \right] \exp \left[ \frac{-\Delta^\circ H_1 \Delta T}{RT_0(T_0 + \Delta T)} \right] \exp(\epsilon_{11}^L X_1^L)
= X_1^L \exp \left[ \frac{\Delta^\circ G_1}{RT_0} - \frac{\Delta^\circ H_1 \Delta T}{RT_0(T_0 + \Delta T)} + (\epsilon_{11}^L X_1^L) \right] \tag{6}
\]

and Eqn. (5) may be written

\[
X_i^\gamma \exp(\epsilon_{1i}^X X_i^\gamma) = X_i^L \exp \left[ \frac{\Delta^\circ G_1^{\gamma-L}}{RT} + \epsilon_{11}^L X_i^L \right] \tag{7}
\]

Substituting for \[\frac{\Delta^\circ G_{2s}}{RT_0}\] in Eqn. (2) and rearranging gives the final equation

\[
\frac{\Delta^\circ G_0}{RT_0} - \frac{\Delta^\circ H_0 \Delta T}{RT_0(T + \Delta T)}
\]

80
\[
- \ln|1 - X_1^-| - \sum_{i=2}^{n} X_i^\gamma| + \ln|1 - X_1^-| - \sum_{i=2}^{n} X_i^L|
\]

\[
+ \frac{\epsilon_{11}^-}{2} (X_1^-)^2 - X_1^\gamma \sum_{i=2}^{n} \epsilon_{i1}^- X_i^\gamma + \frac{\epsilon_{11}^L}{2} (X_1^L)^2 - X_1^L \sum_{i=2}^{n} \epsilon_{i1}^L X_i^L = 0 \tag{8}
\]

\(X_1^\gamma\) and \(X_1^\gamma\) are found from (6) and (7) respectively.
APPENDIX 3: PERITECTIC PROGRAM
1 FTVSCLR %H% DATA=.DATA NAG OUTPUT=.OUT
2 C
3 C PROGRAM TO CALCULATE THE PERITECTIC REGION OF THE
4 C IRON-CARON PHASE DIAGRAM FOR ANY GIVEN LOW ALLOY STEEL.
6 C ELEMENTS MUST BE PLACED IN THE DATASET IN THE ORDER:
7 C Mn Si Ni Cr Mo Cu V Nb W Co
8 C
9 IMPLICIT DOUBLE PRECISION (T)
10 DOUBLE PRECISION A(10),AC,Al(10),B(10,5),C,C6,CAF,CF,CLIQ,D(10,6)
11 DOUBLE PRECISION DAT(10),DELTAT,DTALPH,DTGAM,E(10,4),FEAF,G,GC,GI
12 DOUBLE PRECISION H,HC,P,Q,R,WTPC,X(10),XX(10),Z,Z6,Z61
13 COMMON /INTER/B
14 COMMON /DELTAl/D
15 COMMON /DELTAl/E
16 COMMON /PARMS/G,R,TO,T,P,CF,Q,GC,GI,HC,H
17 INTEGER ANS,COUNT,COUNTA,DUMMY,FLAG I,FLAG2,S43,S54,S91
18 COUNTA = 2
19 R = 1.9858D0
20 C cal/mol/K
21 DATA C, SUM, DELTAT/0.0D0, 0.0D0, 0.0D0/
22 DATA TEMP, TI, VO.0D0, O.0D0, 0.0D0/
23 **************************************************************
24 C
25 C INTRODUCTION
26 C
27 WRITE(6,101)
28 WRITE(6,51)
29 READ(5,*) (DAT(I),I=1,10)
30 IF (ADD(DAT).EQ.0.0D0) THEN
31 WRITE(6,159)
32 ELSE
33 WRITE(6,160)
34 IF (DAT(1).NE.0.0D0) WRITE(6,161)DAT(1)
35 IF (DAT(2).NE.0.0D0) WRITE(6,162)DAT(2)
36 IF (DAT(3).NE.0.0D0) WRITE(6,163)DAT(3)
37 IF (DAT(4).NE.0.0D0) WRITE(6,164)DAT(4)
38 IF (DAT(5).NE.0.0D0) WRITE(6,165)DAT(5)
39 IF (DAT(6).NE.0.0D0) WRITE(6,166)DAT(6)
40 IF (DAT(7).NE.0.0D0) WRITE(6,167)DAT(7)
41 IF (DAT(8).NE.0.0D0) WRITE(6,168)DAT(8)
42 IF (DAT(9).NE.0.0D0) WRITE(6,169)DAT(9)
43 IF (DAT(10).NE.0.0D0) WRITE(6,170)DAT(10)
44 ENDIF
45 WRITE(6,51)
46 101 FORMAT(1X,76(1H-),/
47 1' Peritectic program by A. A. B. Sugden.',/
48 2' This program calculates the phase boundaries of a given low allo
49 3y steel from',/
50 4' 0 up to 5wt%C at appropriate intervals. This is done using the t
51 5hermodynastic',/
52 6' formulae developed by Kirkaldy, Thomson, et al. Partition coeffi
53 7cients for',/
54 8' the liquidus line are given for carbon and the solute elements.
55 9')
56 159 FORMAT(' Pure iron')
57 160 FORMAT(' The steel contains:')
58 161 FORMAT(F5.2,' wt% manganese')
59 162 FORMAT(F5.2,' wt% silicon')
60 163 FORMAT(F5.2,' wt% nickel')
61 164 FORMAT(F5.2,' wt% chromium')
62 165 FORMAT(F5.2,' wt% molybdenum')
63 166 FORMAT(F5.2,' wt% copper')
64 167 FORMAT(F5.2,' wt% vanadium')
65 168 FORMAT(F5.2,' wt% niobium')
66 169 FORMAT(F5.2,' wt% tungsten')
67 170 FORMAT(F5.2,' wt% cobalt')
68 **************************************************
69 C
70 C MAIN PROGRAM
71 C
72 DO 19 MM = 1,9
73 C
74 C 1ST LOOP
75 C
76 K=MM
77 IF (K.EQ.2 .OR. K.EQ.8) GOTO 19
78 IF (K.GT.1) WRITE(6,51)
79 IF (K.GT.6) COUNT = 789
80 CALL FIRST(K)
81 DO 1 I = 1,10
82 1 XX(I) = DAT(I)
83 DUMMY = 0
84 2 C6 = 0.0D0
85 NUM = 0
86 C
87 C INITIALIZATION FOR K = 6
88 C
89 IF (COUNT.EQ.-1 .AND. DUMMY.EQ.0) K = 6
90 COUNT = 0
91 FLAG2 = 1
92 DTGAM = 0.0D0
93 Z61 = 1.0D2
94
95 IF (K.EQA) THEN
96 S43 = 3
97 K = K - 1
98 ENDIF
99
100 IF (K.EQ.7) THEN
101 CLIQ = -1.0D0
102 K = K - 6
103 ELSE
104 CLIQ = 5.3D-1
105 ENDIF
106
107 IF (K.EQ.9) THEN
108 S91 = 3
109 K = K - 2
110 GOTO 2
111 ENDIF
112
113 IF (S54.EQ.3) GOTO 3
114 IF (DUMMY.NE.3) THEN
115 IF (K.NE.5) WRITE(6,52)
116 IF (K.NE.6 .AND. K.NE.5) WRITE(6,55)

117 ENDIF
118 3 CONTINUE
119 DO 17 N = 1,70
120 C
121 C 2ND LOOP
122 C
123 IF (COUNT.EQ.-1 .OR. COUNT.EQ.12) GOTO 17
124 IF (K.EQ.5 .AND. NUM.EQ.3) GOTO 17
125 C = (N-1)*0.01
126 4 CONTINUE
127 IF (K.EQ.3 .OR. NUM.EQ.1) C = C*0.1
128 5 WTPC = C + ADD(XX)
129 IF (WTPC.GT.5.0) THEN
130 WRITE(6,52)
131 WRITE(6,54)
132 GOTO 18
133 ENDIF
134 C
135 C CALCULATION OF MOLE FRACTIONS
136 C
137 FEA = (1.0D2-WTPC)/5.58D1
138 CAF = C/1.2D1
139 DO 6 M = 1,10
140 6 X(M) = XX(M)/B(M,1)
141 TAF = FEA + CAF + ADD(X)
142 CF = CAF/TAF
143 DO 7 M = 1,10
144 7 X(M) = X(M)/TAF
145
146 IF (K.EQ.1) THEN
147 IF (C.LE.CLIQ) THEN
148 IF (NUM.EQ.1) THEN
149 TO = 1.809D3 - 2.013D2*C - 2.949D3*C*C
150 ELSE
151 TO = 1.809D3 - 2.956D1*C - 8.6D1*C*C
152 ENDIF
153 H = 3.3D3
154 C cal/mol
155 HC = -2.13D4
156 T = TO
157 8 CONTINUE
158 GC = 6.3D0*T - 2.13D4
159 GOTO 10
160 ELSE
161 IF (S91.EQ.3) THEN
162 TO = 1.783D3 - 1.640D2*C - 1.674D1*C*C
163 ELSE
164 TO = 1.799D3 - 5.432D1*C - 7.869D0*C*C
165 ENDIF
166 T = TO
167 H = 3.6D3
168 HC = -5.36D3
169 9 CONTINUE
170 GC = 6.0D-1*T - 5.36D3
171 ENDIF
172 10 AC = DEXP(GC/(R*TO)+(3.89D-l+7.81D3(f)*CF)
173 AC = AC/(1+(8.91D3(f)*CF*DEXP(GC/(R*TO)))
174 ENDIF
175
176 IF (K.EQ.3) THEN
177 IF (DUMMY.EQ.0) THEN
178 K = K + 3
179 DUMMY = 3
180 GOTO 5
181 ENDIF
182 DUMMY = 8
183 IF (S43.EQ.3) THEN
184 TO = 1.667D3 + 1.122D3*C
185 C
186 C REF: METALS HANDBOOK, 1978
187 C
188 ELSE
189 TO = 1.667D3 + 9.81D2*C - 2.17D3*C*C
190 ENDIF
191 H = 2.0D2
192 HC = -1.5325D4
193 T = TO
194 CF = 0
195 12 G = -1.36D-1*T + 2.258D2
196 GC = -7.686D0*T + 1.5325D4
197 ENDIF
198
199 IF (K.EQ.5) THEN
200 IF (DUMMY.EQ.0 .AND. COUNT.NE.11) THEN
201 K = K + 1
202 DUMMY = 5
203 GOTO 5
204 ENDIF
205 DUMMY = -1
206 K = K - 4
207 NUM = NUM + 1
208 GOTO 5
209 ENDIF
210
211 IF (K.EQ.6) THEN
212 K = K - 5
213 C = CLIQ
214 COUNT = 3
215 GOTO 5
216 13 IF (DELTAT.EQ.0.0D0) THEN
217 COUNT = -1
218 GOTO 15
219 ELSE
220 FLAG1 = COUNT/COUNTA
221 IF (FLAG1.NE.FLAG2) THEN
222 DTGAM = DELTAT
223 IF (DELTAT.GT.0.0D0) THEN
224 CLIQ = CLIQ - 5.0D-3
225 ELSE
226 CLIQ = CLIQ + 5.0D-3
227 ENDIF
228 C = CLIQ
229 ELSE
230 DTALPH = DELTAT
231 C = CLIQ + 1.0D-3
232 ENDIF
233 Z6 = DTALPH - DTGAM
234 \( Z6 = \text{DABS}(Z6) \)
235 IF (\( Z6 \geq Z61 \)) THEN
236 \( T = T - Z6 \)
237 \( \text{COUNT} = -1 \)
238 GOTO 15
239 ENDIF
240 \( \text{COUNT} = \text{COUNT} + 1 \)
241 \( \text{FLAG2} = \text{FLAG1} \)
242 \( Z61 = Z6 \)
243 GOTO 5
244 ENDIF
245 ENDIF
246
247 \( \text{SUM} = 0.0D0 \)
248 \( \text{DELTAT} = 0.0D0 \)
249 DO 14 \( M = 1,10 \)
250 C
251 C 3RD LOOP
252 C
253 IF (\( X(M) = 0 \)) THEN
254 \( A(M) = 0.0D0 \)
255 \( \text{AI}(M) = 1.0D0 \)
256 GOTO 14
257 ENDIF
258 IF (\( K = 1 \)) THEN
259 IF (\( C \leq C_{\text{Liq}} \)) THEN
260 \( Q = 0.0D0 \)
261 ELSE
262 Q = \( B(M,4) + B(M,5) \)
263 ENDIF
264 ENDIF
265 \( P = B(M,2) + B(M,3) \)
266 IF (\( C \leq C_{\text{Liq}} \)) THEN
267 \( G = -2646 + 39.1693*T - 5.27*T*D\log(T) + 0.001*T*T - 0.136*T + 2.258D2 \)
268 \( GI = -(D(M,5) + D(M,6)*T) \)
269 ELSE
270 \( G = -2646 + 39.1693*T - 5.27*T*D\log(T) + 0.001*T*T \)
271 \( GI = -(D(M,1) + (D(M,2) + D(M,3)*D\log(T) + D(M,4)*T)*T) \)
272 ENDIF
273 C
274 C CALCULATION OF SOLUTE PARTITION COEFFICIENTS FOR THE LIQUIDUS
275 C
276 AI(M) = DEXP(GI/(R*TO)+P*CF)
277 AI(M) = AI(M)/(1+Q*CF*DEXP(GC/(R*TO)))
278 ENDIF
279
280 IF (K.EQ.3) THEN
281 P = 0.0D0
282 Q = B(M,4) + B(M,5)/T
283 IF (M.EQ.1) THEN
284 GI = 6.5D2 - 3.05D-1*T
285 ELSE
286 IF (M.EQ.3) THEN
287 GI = 3.0D2
288 ELSE
289 IF (M.EQ.6) THEN
290 GI = 1.45D3 - 8.0D-1*T
291 ELSE
292 GI = -(E(M,1)+(E(M,2)+E(M,3)*T+E(M,4)*DLOG(T))*T)
293 C
294 C NOTE MINUS SIGN
295 C
296 ENDIF
297 ENDIF
298 ENDIF
299 ENDIF
300
301 CALL EQN(A(M),K,C,CLIQ)
302 SUM = SUM + X(M)*A(M)
303 14 CONTINUE
304 DELTAT = SUM*R*TO*TO
305 T = TO + DELTAT
306 Z = TT - T
307 Z = DABS(Z)
308 IF (Z.LT.0.5D0) GOTO 15
309 TT = T
310 IF (K.EQ.1) THEN
311 IF (C.LE.CLIQ) THEN

89
312 GOTO 8
313 ELSE
314 GOTO 9
315 ENDIF
316 ENDIF
317 IF (K.EQ.3) GOTO 12
318 15 CONTINUE
319
320 IF (K.EQ.3) THEN
321 IF (T.GT.TEMP) THEN
322 IF (COUNT.EQ.0) THEN
323  C = (N-1)*0.02 - 0.01
324 COUNT = 11
325 GOTO 5
326 ELSE
327 IF (NUM.NE.2) THEN
328 WRITE(6,52)
329 IF (S43.EQ.3) THEN
330 WRITE(6,59)C-5.0D-3
331 ELSE
332 WRITE(6,58)C-5.0D-3
333 ENDIF
334 IF (DUMMY.EQ.8) THEN
335 WRITE(6,60)TEMP-273
336 ELSE
337 WRITE(6,60)TEMP
338 ENDIF
339 COUNT = 12
340 GOTO 17
341 ENDIF
342 ENDIF
343 ELSE
344 IF (COUNT.EQ.11) THEN
345 IF (NUM.NE.2) THEN
346 WRITE(6,52)
347 IF (S43.EQ.3) THEN
348 WRITE(6,59)C+5.0D-3
349 ELSE
350 WRITE(6,58)C+5.0D-3

351 ENDIF
352 IF (DUMMY.EQ.8) THEN
353 WRITE(6,60)TEMP-273
354 ELSE
355 WRITE(6,60)TEMP
356 ENDIF
357 COUNT = 12
358 GOTO 17
359 ENDIF
360 ENDIF
361 ENDIF
362 ENDIF
363
364 IF (COUNT.GE.3) GOTO 13
365 IF (COUNT.EQ.-1) THEN
366 IF (DUMMY.EQ.0) THEN
367 WRITE(6,60)T-273
368 WRITE(6,61)C
369 ELSE
370 TEMP = T
371 ENDIF
372 GOTO 17
373 ENDIF
374 IF (K.EQ.3 .AND. S54.EQ.3) GOTO 17
375 IF (K.EQ.3 .AND. S93.NE.3) THEN
376 IF (NUM.NE.2) THEN
377 WRITE(6,62)C,T-273
378 ELSE
379 WRITE(6,63)C,T-273
380 ENDIF
381 ELSE
382 IF (S91.EQ.3 .AND. N.EQ.1) GOTO 17
383 IF (NUM.EQ.1) THEN
384 IF (T.LT.TEMP) THEN
385 WRITE(6,52)
386 WRITE(6,57)
387 COUNT = -1
388 GOTO 17
389 ELSE
390 WRITE(6,62)C, T-273
391 ENDIF
392 ELSE
393 C
394 C K = 1
395 C
396 WRITE(6,63)C, T-273
397 IF (K.EQ.1) THEN
398 IF (CLIQ.EQ.-1.0D0 .OR. S91.EQ.3) GOTO 17
399 WRITE(6,64)AC
400 DO 16 I = 1,10
401 IF (AI(I).EQ.1.0D0) GOTO 16
402 IF (I.LT.9) THEN
403 WRITE(6,65)I+1, AI(I)
404 ELSE
405 WRITE(6,66)I+1, AI(I)
406 ENDIF
407 16 CONTINUE
408 ENDIF
409 ENDIF
410 ENDIF
411 17 CONTINUE
412 IF (K.EQ.1 .OR. K.EQ.5) THEN
413 IF (DUMMY.EQ.-1) GOTO 18
414 ENDIF
415 IF (DUMMY.NE.0 .AND. DUMMY.NE.8) THEN
416 IF (DUMMY.EQ.3) K = K + 2
417 IF (DUMMY.EQ.5) K = K + 4
418 GOTO 2
419 ENDIF
420 18 CONTINUE
421 19 CONTINUE
422 STOP
423
424 51 FORMAT(1X,63(IH-))
425 52 FORMAT(IX)
426 54 FORMAT(' The sum of the alloy components should not exceed 5wt%')
427 55 FORMAT(' WT%C : T/Centigrade')
428 57 FORMAT(' Solidus ends.')
92
The peritectic point is at \( F_{\text{peritecic}} \) wt%.
The maximum solubility of the carbon in delta-iron is \( F_{\text{max solubility}} \) wt%.
The peritectic line is at approx. \( F_{\text{peritectic line}} \) Centigrade.
The line stops at \( F_{\text{line stop}} \) wt%.

C DATA FOR ALLOYING ELEMENT INTERACTION PARAMETERS

C

BLOCK DATA ETA

COMMON /INTER/B

DOUBLE PRECISION B(10,5)

DATA((B(M,J),J=1,5),M=1,10)/

C5.49D1,0.0D0,-5.06D3,0.0D0,-5.07D3,
C2.81D1,4.28D-1,1.874D4,4.84D0,-7.37D3,
C5.87D1,0.0D0,5.34D3,-2.2D0,7.6D3,
C5.20D1,0.0D0,-9.5D3,2.44D1,-3.84D4,
C9.59D1,0.0D0,-7.49D3,3.855D0,-1.787D4,
C6.35D1,0.0D0,7.586D3,0.0D0,4.2D3,
C5.09D1,0.0D0,-3.01D4,0.0D0,-2.466D4,
C9.29D1,0.0D0,-4.6615D4,0.0D0,-2.877D4,
C1.838D2,0.0D0,-1.223D4,2.34D1,-3.6214D4,
C5.89D1,0.0D0,3.55D3,0.0D0,2.8D3/

END

C

DATA FOR ALLOYING ELEMENT FREE ENERGY CHANGES (DELTA G(I))

COMMON /DELTA1/ D

DOUBLE PRECISION D(10,6)

DATA((D(M,J),J=1,6),M=1,10)/
468 C-2.86D3,2.03D0,0.00D0,0.00D0,-2213.00D0,1.727D0,
469 C2.23D3,3.49D1,-4.7244D0,0.00D0,8.2D3,-3.90D0,
470 C7.9D2,6.4D1,1.00D0,0.00D0,2.12D3,3.8D1,
471 C4.23D3,-6.89D0,6.568D-1,1.00D0,4.6D3,-2.19D0,
472 C7.165D3,-2.14D0,0.00D0,0.00D0,6.6D3,-2.29D0,
473 C3.15D3,-1.39D0,0.00D0,0.00D0,1.2D3,0.00D0,
474 C-3.25703,1.1501,0.000,-5.10-3,5.103,-2.300,
475 C5.503,-2.300,0.000,0.000,5.503,-2.300,
476 C1.004,-3.500,0.000,0.000,7.503,-3.6500,
477 C-3.9503,2.1900,0.000,0.000,-3.503,2.1900/
478 END

480 C
481 C DATA FOR ALLOYING ELEMENT FREE ENERGY CHANGES (DELTA G(I))
482 C [FERRITE-AUSTENITE TRANSFORMATION]
483 C
484 BLOCK DATA DGI2
485 COMMON /DELTA2/E
486 DOUBLE PRECISION E(10,4)
487 DATA((E(M,J),J=1,4),M=1,10)/
488 C-1.76D3,-4.7D-1,1.00D0,0.00D0,
489 C-5.964D3,3.8799D-1,0.00D0,-4.7244D0,
490 C-5.607D3,-3.8D-1,1.00D0,0.00D0,
491 C-3.67D2,-4.656D0,0.00D0,6.568D-1,
492 C5.65D2,1.5D-1,1.00D0,0.00D0,
493 C-2.55D4,4.1183D1,-1.7D-1,1.00D0,
494 C-8.357D3,1.38D1,-5.1D-3,0.00D0,
495 C1.434D1,-1.3D-3,0.00D0,0.00D0,
496 C2.5D3,1.5D-1,1.00D0,0.00D0,
497 C0.0D0,0.00D0,0.00D0,0.00D0/
498 END

499

500 SUBROUTINE FIRST(L)
501 IF (L.EQ.1) WRITE(6,1)
502 IF (L.EQ.3) WRITE(6,3)
503 IF (L.EQ.4) WRITE(6,4)
504 IF (L.EQ.5) WRITE(6,5)
505 IF (L.EQ.6) WRITE(6,6)
506 IF (L.EQ.7) WRITE(6,7)
IF (L.EQ.9) WRITE(6,9)
RETURN
1 FORMAT (' Liquidus. ')
3 FORMAT (' Austenite/Delta+Austenite line. ')
4 FORMAT (' Delta/Delta+Austenite line. ')
5 FORMAT (' Delta solidus. ')
6 FORMAT (' Peritectic line. ')
7 FORMAT (' Solidification as primary austenite. ')
9 FORMAT (' Austenite solidus. ')
END

DOUBLE PRECISION FUNCTION ADD(Y)
DOUBLE PRECISION Y(10)
ADD = 0.0D0
DO 4 I = 1,10
ADD = ADD + Y(I)
RETURN
END

******************************************************************************
C
C MAIN CALCULATION
C
SUBROUTINE EQN (F16,NO,CC,CQIL)
IMPLICIT DOUBLE PRECISION (F)
DOUBLE PRECISION G,R,TO,T,P,CF,Q,GC,GI,HC,H
DOUBLE PRECISION CC,CQIL,EG11,EL11
COMMON /PARMS/G,R,TO,T,P,CF,Q,GC,GI,HC,H
C
C SET CARBON-CARBON INTERACTION PARAMETERS
C
IF (NO.EQ.1) THEN
IF (CC.LE.CQIL) THEN
EG11 = 0.0D0
ELSE
EG11 = 8.91D3/f
ENDIF
EL11 = 3.89D-1 + 7.81D3/f
ENDIF
IF (NO.EQ.2) THEN
IF (NO.EQ.3) THEN
EG11 = 8.91D3/T
EL11 = 0.0D0
ENDIF

IF (NO.EQ.3) THEN
EG11 = 8.91D3/T
EL11 = 0.0D0
ENDIF

F1 = G1/(R*TO) + P*CF
F2 = GC/(R*TO)
F3 = 1 + Q*CF*DEXP(F2)
F4 = GC/(R*TO) + (EL11)*CF
F5 = 1 + EG11*CF*DEXP(F2)
F6 = DEXP(F1)/F3
F7 = DEXP(F4)/F5
F8 = 1+CF*(1-CF)*(P-Q*F6*F7)
F9 = G/(R*TO*TO)
F10 = CF*CF/2*((EL11)-(EG11*F7*F7))
F11 = DEXP(F4)*CF*HC/F5
F12 = (1-CF)*H
F13 = F9 - F10
F14 = F11+F12*DEXP(F13)
F15 = F8*DEXP(F13)
F16 = (F6-F15)/F14
RETURN
END

%
APPENDIX 4: STRENGTHENING PROGRAM

1 ITVSCLR PROGRAM=%H% DATA=.DATA NAG OUTPUT=.OUT:TWO
2 C
3 C PROGRAM TO CALCULATE SOLID SOLUTION STRENGTHENING
4 C AND STRENGTHENING DUE TO PURE ANNEALED IRON
5 C AS A FUNCTION OF TEMPERATURE AND STRAIN RATE.
8 C ENTER THE FOLLOWING VARIABLES (COMPOSITIONS IN WT%):
9 C TEMPERATURE, Ni, Mn, Si, Cr, Co, V,
10 C Mo, Al, Nb, XX, P, C, N, B, STRAIN RATE,
11 C TEMPERATURE RANGE: 100 TO 750K.
12 C STRAIN RATE RANGE: 5X10^-6 TO 10^-2/S (AN APPROPRIATE DEFAULT
13 C SETTING IS CHOSEN).
14 C XX IS A DUMMY VARIABLE, AND MEANS THAT ANOTHER ELEMENT MAY
BE
15 C ADDED VERY EASILY.
16 C
17 IMPLICIT REAL*8(A-H,O-$)
18 DOUBLE PRECISION BLOCK(20,500)
19 DIMENSION C(15),DAT(15),DELSIG(15),NUM(15),Q(15)
20 DIMENSION ITLSUM(500),YLDSTR(500)
21 COMMON/TOT/ITLSUM
22 COMMON/ARM/SRATE
23 COMMON/PARS/C,DAT,T
24 DATA DELSIG(12), DS, P/0.0D0, 0.0D0, 0.0D0/,
25 DATA Q/15*0.0D0/,NUM/15*0/
26
27 READ(5,*) I21,(BLOCK(J,1),J=1,20),I=1,I21
28 DO 88 I22 = 1,I21
29 T = BLOCK(1,I22)
30 DO 77 I23 = 2,16
31 N = I23 - 1
32 77 DAT(N) = BLOCK(I23,I22)
33 SRATE = BLOCK(17,I22)
34 T = T + 2.73D2
35 CALL ATOMFR
36 CALL IFDS(C,DELSIG,NUM)
37 CALL ELSEDS(Q)
38 IF (DAT(12).GT.0.0D0) CALL PHOS(C(12),DELSIG(12),NUM(12))
39 CALL RESULT(DELSIG,Q,NUM,I22)
40 WRITE(6,101)
41 YLDSTR(I22) = (BLOCK(18,I22)*9.80665D0)/3.0D0
42 C
43 C CALCULATION OF YIELD STRENGTH FROM HARDNESS
44 C
45 CALL NCCALC(YLDSTR(I22), BLOCK(19,I), BLOCK(20,I))
46 88 CONTINUE
47 WRITE(6,105)121
48 DO 4 I = 1,121
49 $MICRO = YLDSTR(I) - TTLSUM(I)
50 4 WRITE(6,110)BLOCK(18,1),YLDSTR(I),TTLSUM(I),
51 &$MICRO,BLOCK(19,1)/1.0D2,BLOCK(20,1)/1.0D2
52 STOP
53 101 FORMAT(1X,50(lH*))
54 105 FORMAT(' SUMMARY:',/
55 &' HV TOTAL/MPA SS+FE/MPA MICRO/MPA VALPHA VACIC
56 &SETS OF DATA'/, 
57 &' ' ————Delete the above for regression analysis——
58 &'——' ,'/, 
59 &'
60 & ',13)
61 110 FORMAT(F8.2,2F12.2,F10.2,2F10.4)
62 END
63 ************************************************************************
64 SUBROUTINE ATOMFR
65 C
66 C CALCULATES ATOM FRACTIONS OF THE ALLOYING ELEMENTS
67 C
68 DOUBLE PRECISION AW(15),C(15),DAT(15),FEAF,T,TAF
69 COMMON/PARMS/C,DAT,T
70 DATA AW(1),AW(2),AW(3)/5.87D1,5.49D1,2.81D1/,
71 * AW(4),AW(5),AW(6),AW(7)/5.2D1,5.89D1,5.09D1,4.79D1/, 
72 * AW(8),AW(9),AW(10),AW(11)/9.59D1,2.7D1,9.3D1,1.0D2/, 
73 * AW(12),AW(13),AW(14),AW(15)/3.1D1,1.2D1,1.4D1,1.08D1/
74 DO 4 I = 1,15
75 4 C(I) = DAT(I)/AW(I)
76 FEAF = (1.0D2-ADD(DAT))/5.58D1
77 TAF = FEAF + ADD(C)
78 DO 6 I = 1,15
79 6 C(I) = C(I)*1.0D2/TAF
80 END
81*****************************************************************************
82 FUNCTION ADD(Y)
83 DOUBLE PRECISION Y(15)
84 ADD = 0.0D0
85 DO 4 I = 1,15
86 4 ADD = ADD + Y(I)
87 RETURN
88 END
89*****************************************************************************
90 SUBROUTINE IFDS(AT,DSI,I1)
91 C
92 C CALCULATES STRENGTHENING DUE TO NI, MN, SI, CR, CO, V, TI, MO, AL, NB AND XX AT 23 DEGC
93 C
94 C
95 DOUBLE PRECISION AT(15),DSI(15),FACTOR(11),LIM(11)
96 INTEGER I1(15)
97 DATA FACTOR(1),FACTOR(2),FACTOR(3)/1.965D1,1.85D1,2.68D1/, 98 * FACTOR(4),FACTOR(5),FACTOR(6)/3.5D0,3.43D0,2.07D0/, 99 * FACTOR(7),FACTOR(8),FACTOR(9)/1.76D1,1.55D1,9.31D0/, 100 * FACTOR(10),FACTOR(11),LIM(1),LIM(2)/0.0D0,0.0D0,2.84D0,2.97D0/, 101 * LIM(3),LIM(4),LIM(5),LIM(6)/5.72D0,6.86D0,5.56D0,1.043D1/, 102 * LIM(7),LIM(8),LIM(9),LIM(10)/1.0D1,1.79D0,5.85D0,1.0D1/, 103 * LIM(11)/1.0D1/
104 C
105 C LIMITS FOR TI AND NB SET AT 10%
106 C
107 DO 5 I = 1,11
108 DSI(I) = FACTOR(I)*AT(I)
109 5 IF (AT(I).GT.LIM(I)) I1(I) = 1
110 END
111*****************************************************************************
112 SUBROUTINE ELSEDS(ELSE)
113 C
114 C CALCULATES STRENGTHENING DUE TO NI, MN, SI, CR, AND CO AT T.NE.23DEGC
115 C
116 TAF = FEAF + ADD(C)
78 DO 6 I = 1,15
79 6 C(I) = C(I)*1.0D2/TAF
116 C
117 DOUBLE PRECISION C(15),DAT(15),T,ELSE(15)
118 COMMON/PARMS/C,DAT,T
119 IF (DAT(1).GT.0.0D0) CALL NICKEL(C(1),T,ELSE(1))
120 IF (DAT(2).GT.0.0D0) CALL MANGAN(C(2),T,ELSE(2))
121 IF (DAT(3).GT.0.0D0) CALL SILICN(C(3),T,ELSE(3))
122 IF (DAT(4).GT.0.0D0) CALL CHROM(C(4),T,ELSE(4))
123 IF (DAT(5).GT.0.0D0) CALL COBALT(C(5),T,ELSE(5))
124 END

125***********************************************************************

126 SUBROUTINE NICKEL(CONC,XARG,DNI)
127 DOUBLE PRECISION K(13),KNI(2,13),C(13),CNI(2,13)
128 DOUBLE PRECISION X(2),Y(2),Al,A2,DNl
129 DATA CN1(1,1),CN1(1,2),CN1(1,3)/-3.86D1,-4.67D1,-6.8D1/,
130 * CN1(1,4),CN1(1,5),CN1(1,6),CN1(1,7)/6.57D1,2.8D1,3.61D1, 1.45D1/,
131 * CN1(1,8),CN1(1,9),CN1(1,10),CN1(1,11)/1.62D1,1.0D0,0.0D0,0.0D0/
132 * .CN1(1,12),CN1(1,13),CN1(1,14),CN1(1,15)/0.0D0,-5.7D1,-4.8D1/,
133 * CN1(1,16),CN1(1,17),CN1(1,18),CN1(1,19)/6.38D1,1.39D2,7.9D1,7.56D1/,
134 * CN1(1,20),CN1(1,21),CN1(1,22)/4.03D1,3.91D1,1.0D0,0.0D0/
135 * .CN1(1,23),CN1(1,24),CN1(1,25),CN1(1,26)/1.0D0,0.0D0,1.0D2,1.0D2/,
136 * KNI(1,1),KNI(1,2),KNI(1,3),KNI(1,4)/0.0D0,0.0D0,0.0D0,0.0D0/
137 * KNI(1,5),KNI(1,6),KNI(1,7),KNI(1,8)/0.0D0,0.0D0,0.0D0,0.0D0/
138 * KNI(1,9),KNI(1,10),KNI(1,11),KNI(1,12)/1.0D0,1.0D2,1.0D2,1.0D2/,
139 * KNI(1,13),KNI(1,14),KNI(1,15),KNI(1,16)/2.5D2,3.4D2,5.8D2,7.5D2/,
140 * KNI(1,17),KNI(1,18),KNI(1,19),KNI(1,20)/7.5D2,7.5D2,7.5D2,1.0D2/,
141 * KNI(1,21),KNI(1,22),KNI(1,23),KNI(1,24)/1.0D2,1.0D2,1.0D2,1.0D2/,
142 * .CN1(2,1),CN1(2,2)/-3.5D1,-1.17D2/
143 DATA NCAP7,IFAIL/13.0/ 
144 DATA X(1),X(2)/1.44D0,2.84D0/
145 C
146 C CALCULATE DNI AT A GIVEN TEMPERATURE FOR TWO CONCENTRATIONS
147 C
148 DO 8 I = 1,2
149 DO 5 J = 1,13
150 K(J) = KNI(I,J)
151 5 C(J) = CN1(I,J) /
152 8 CALL E02BBF(NCAP7,K,C,XARG,Y(I),IFAIL)
153 C
154 C EXPRESS DNI AS A FUNCTION OF CONCENTRATION
155 C
156 A2 = (Y(2)/X(2)-Y(1)/X(1))/(X(2)-X(1))
157 A1 = Y(1)/X(1) - A2*X(1)
158 DNI = A1*CONC + A2*CONC*CONC
159 END
160 ************************************************************************
161 SUBROUTINE MANGAN(CONC,XARG,DMN)
162 DOUBLE PRECISION K(13),KMN(2,13),C(13),CMN(2,13)
163 DOUBLE PRECISION X(2),Y(2),A1,A2,DMN
164 DATA CMN(1,1),CMN(1,2),CMN(1,3)/-1.25D1,-6.22D1,-5.16D1/,
165 * CMN(1,4),CMN(1,5),CMN(1,6)/-1.01D2,7.02D1,5.66D1/,
166 * CMN(1,7),CMN(1,8),CMN(1,9)/5.12D1,3.07D1,2.585D1/,
167 * CMN(1,10),CMN(1,11),CMN(1,12),CMN(1,13)/0.00D0,0.00D0,0.00D0/, 
168 * KMN(1,1),KMN(1,2),KMN(1,3),KMN(1,4)/1.0D2,1.0D2,1.0D2,1.0D2/, 
169 * KMN(1,5),KMN(1,6),KMN(1,7),KMN(1,8)/1.3D2,1.9D2,2.3D2,3.2D2/, 
170 * KMN(1,9),KMN(1,10),KMN(1,11)/5.6D2,7.5D2,7.5D2/, 
171 * KMN(1,12),KMN(1,13)/7.5D2,7.5D2/ 
172 DATA CMN(2,1),CMN(2,2),CMN(2,3)/-5.02D1,-4.975D1,-1.46D2/, 
173 * CMN(2,4),CMN(2,5),CMN(2,6)/9.02D1,1.135D2,6.94D1/, 
174 * CMN(2,7),CMN(2,8),CMN(2,9)/6.95D1,6.905D1,6.17D1/, 
175 * CMN(2,10),CMN(2,11),CMN(2,12),CMN(2,13)/0.00D0,0.00D0,0.00D0/ 
176 * KMN(2,1),KMN(2,2),KMN(2,3),KMN(2,4)/1.0D2,1.0D2,1.0D2,1.0D2/, 
177 * KMN(2,5),KMN(2,6),KMN(2,7),KMN(2,8)/1.625D2,2.0D2,3.0D2,4.875D2/ 
178 * KMN(2,9),KMN(2,10),KMN(2,11)/6.5D2,7.5D2,7.5D2/, 
179 * KMN(2,12),KMN(2,13)/7.5D2,7.5D2/ 
180 DATA NCAP7,IFAIL/13,0/ 
181 DATA X(1),X(2)/1.54D0,2.97D0/ 
182 DO 8 I = 1,2 
183 DO 5 J = 1,13 
184 K(J) = KMN(I,J) 
185 C(J) = CMN(I,J) 
186 8 CALL E02BBF(NCAP7,K,C,XARG,Y(I),IFAIL) 
187 A2 = (Y(2)/X(2)-Y(1)/X(1))/(X(2)-X(1)) 
188 A1 = Y(1)/X(1) - A2*X(1) 
189 DMN = A1*CONC + A2*CONC*CONC 
190 END 
191 ************************************************************************
192 SUBROUTINE SILICON(CONC,XARG,DSI) 
193 DOUBLE PRECISION K(13),KSI(3,13),C(13),CSI(3,13),FIT,XARG
194 DOUBLE PRECISION X(4), Y(4), W(4), WORK1(3,4), WORK2(2,3)
195 DOUBLE PRECISION A(3,3), S(3), B(3), CONC, DSI, XCAP
196 INTEGER M, KPLUS1, NRROWS, IFAIL, NPLUS1
197 DATA CSI(1,1), CSI(1,2), CSI(1,3)/-3.575D1, -7.84D1, -3.97D1/,
198 * CSI(1,4), CSI(1,5), CSI(1,6)/-1.245D2, 5.53D1, 7.71D1/,
199 * CSI(1,7), CSI(1,8), CSI(1,9)/4.75D1, 5.205D1, 4.04D1/
200 * CSI(1,10), CSI(1,11), CSI(1,12), CSI(1,13)/0.0D0, 0.0D0, 0.0D0, 0.0D0/
201 * KSI(1,1), KSI(1,2), KSI(1,3), KSI(1,4)/1.0D2, 1.0D2, 1.0D2, 1.0D2/, 202 * KSI(1,5), KSI(1,6), KSI(1,7), KSI(1,8)/1.3D2, 1.8D2, 2.3D2, 2.9D2/, 203 * KSI(1,9), KSI(1,10), KSI(1,11)/4.6D2, 7.5D2, 7.5D2/, 204 * KSI(1,12), KSI(1,13)/7.5D2, 7.5D2/
205 DATA CSI(2,1), CSI(2,2), CSI(2,3)/-3.69D1, -4.93D0, -1.06D2/, 206 * CSI(2,4), CSI(2,5), CSI(2,6)/1.065D2, 1.795D2, 9.54D1/, 207 * CSI(2,7), CSI(2,8), CSI(2,9)/1.205D2, 8.37D1, 9.25D5D1/, 208 * CSI(2,10), CSI(2,11), CSI(2,12), CSI(2,13)/0.0D0, 0.0D0, 0.0D0, 0.0D0/ 209 * KSI(2,1), KSI(2,2), KSI(2,3), KSI(2,4)/1.0D2, 1.0D2, 1.0D2, 1.0D2/, 210 * KSI(2,5), KSI(2,6), KSI(2,7), KSI(2,8)/1.3D2, 2.0D2, 2.75D2, 4.125D2/, 211 * KSI(2,9), KSI(2,10), KSI(2,11), KSI(2,12)/6.0D2, 7.5D2, 7.5D2, 7.5D2/, 212 * KSI(2,13)/7.5D2/
213 DATA CSI(3,1), CSI(3,2), CSI(3,3)/8.87D1, 1.39D2, 2.41D2/, 214 * CSI(3,4), CSI(3,5), CSI(3,6)/3.28D2, 3.04D2, 2.5D2/, 215 * CSI(3,7), CSI(3,8), CSI(3,9)/2.15D2, 1.79D2, 1.68D2/, 216 * CSI(3,10), CSI(3,11), CSI(3,12), CSI(3,13)/0.0D0, 0.0D0, 0.0D0, 0.0D0/ 217 * KSI(3,1), KSI(3,2), KSI(3,3), KSI(3,4)/1.0D2, 1.0D2, 1.0D2, 1.0D2/, 218 * KSI(3,5), KSI(3,6), KSI(3,7), KSI(3,8)/2.2D2, 2.8D2, 3.1D2, 4.0D2/, 219 * KSI(3,9), KSI(3,10), KSI(3,11), KSI(3,12)/5.75D2, 7.5D2, 7.5D2, 7.5D2/, 220 * KSI(3,13)/7.5D2/
221 DATA NCAP7, IFAIL/13, 0/
222 DATA X(1), X(2), X(3), X(4), Y(1)/0.0D0, 1.38D0, 2.8D0, 5.72D0, 0.0D0/, 223 * W(1), W(2), W(3), W(4)/1.0D3, 1.0D0, 1.0D0, 1.0D0/
224 DATA M, KPLUS1, NRROWS, NPLUS1/4, 3, 3, 3/
225 DO 8 I = 1, 3
226 DO 5 J = 1, 13
227 K(J) = KSI(I, J)
228 5 C(J) = CSI(I, J)
229 CALL E02BBF(NCAP7, K, C, XARG, FIT, IFAIL)
230 8 Y(I+1) = FIT
231 CALL E02ADF(M, KPLUS1, NRROWS, X, Y, W, WORK1, WORK2, A, S, IFAIL)
232 DO 12 I = 1, 3

102
233 12 B(I) = A(3,I)
234 XCAP = (2.0D0*CONC-X(4))/X(4)
235 CALL E02AEF(NPLUS1,B,XCAP,DSI,IFAIL)
236 END
237************************************************************************
238 SUBROUTINE CHROM(CONC,XARG,DCR)
239 DOUBLE PRECISION K(13),KCR(3,13),C(13),CCR(3,13),FIT,XARG
240 DOUBLE PRECISION X(4),Y(4),W(4),WORK1(3,4),WORK2(2,3)
241 DOUBLE PRECISION A(3,3),S(3),B(3),CONC,DCR,XCAP
242 INTEGER M,KPLUS1,NROWS,IFAIL,NPLUS1
243 DATA CCR(1,1),CCR(1,2),CCR(1,3)/3.47D1,2.815D1,4.1D1/, 244 * CCR(1,4),CCR(1,5),CCR(1,6),CCR(1,7)/-1.3D1,1.56D1,1.02D1,4.38D1/ 245 * CCR(1,8),CCR(1,9),CCR(1,10)/5.21D0,1.6D0,0.0D0/, 246 * CCR(1,11),CCR(1,12),CCR(1,13),KCR(1,1)/0.0D0,0.0D0,0.0D0,1.0D2/, 247 * KCR(1,2),KCR(1,3),KCR(1,4),KCR(1,5)/1.0D2,1.0D2,1.0D2,1.7D2/, 248 * KCR(1,6),KCR(1,7),KCR(1,8),KCR(1,9)/2.1D2,2.6D2,3.0D2,4.8D2/, 249 * KCR(1,10),KCR(1,11),KCR(1,12)/7.5D2,7.5D2,7.5D2/, 250 * KCR(1,13)/7.5D2/
251 DATA CCR(2,1),CCR(2,2),CCR(2,3)/5.71D1,5.176D1,3.55D1/, 252 * CCR(2,4),CCR(2,5),CCR(2,6)/2.27D1,1.36D1,7.87D0/, 253 * CCR(2,7),CCR(2,8),CCR(2,9)/9.57D0,6.95D0,7.185D0/, 254 * CCR(2,10),CCR(2,11),CCR(2,12),CCR(2,13)/0.0D0,0.0D0,0.0D0,0.0D0/ 255 * KCR(2,1),KCR(2,2),KCR(2,3),KCR(2,4)/1.0D2,1.0D2,1.0D2,1.0D2/, 256 * KCR(2,5),KCR(2,6),KCR(2,7),KCR(2,8)/1.3D2,1.9D2,3.143D2,4.25D2/, 257 * KCR(2,9),KCR(2,10),KCR(2,11),KCR(2,12)/6.0D2,7.5D2,7.5D2,7.5D2/, 258 * KCR(2,13)/7.5D2/
259 DATA CCR(3,1),CCR(3,2),CCR(3,3)/1.08D-1,5.96D0,1.45D1/, 260 * CCR(3,4),CCR(3,5),CCR(3,6)/1.42D0,1.07D0,5.76D1/, 261 * CCR(3,7),CCR(3,8),CCR(3,9)/2.12D1,3.5D1,1.61D1/, 262 * CCR(3,10),CCR(3,11),CCR(3,12),CCR(3,13)/0.0D0,0.0D0,0.0D0,0.0D0/ 263 * KCR(3,1),KCR(3,2),KCR(3,3),KCR(3,4)/1.0D2,1.0D2,1.0D2,1.0D2/, 264 * KCR(3,5),KCR(3,6),KCR(3,7),KCR(3,8)/1.5D2,2.1D2,2.3D2,2.8D2/, 265 * KCR(3,9),KCR(3,10),KCR(3,11)/3.3D2,7.5D2,7.5D2/, 266 * KCR(3,12),KCR(3,13)/7.5D2,7.5D2/
267 DATA NCAP7,IFAIL/13,0/
268 DATA X(1),X(2),X(3),X(4),Y(1)/0.0D0,1.65D0,3.1D0,6.86D0,0.0D0/, 269 * W(1),W(2),W(3),W(4)/1.0D3,1.0D0,1.0D0,1.0D0/
270 DATA M,KPLUS1,NROWS,NPLUS1/4,3,3,3/
271 DO 8 I = 1,3
103
DO 5 J = 1,13
K(J) = KCR(I,J)
5 C(J) = CCR(I,J)
CALL E02BBF(NCAP7,K,C,XARG,FIT,IFAIL)
8 Y(I+1) = FIT
CALL E02ADF(M,KPLUS1,NROWS,X,Y,W,WORK1,WORK2,A,S,IFAIL)
DO 12 I = 1,3
B(I) = A(3,I)
XCAP = (2.0D0*CONC-X(4))/X(4)
CALL E02AEF(NPLUS1,B,XCAP,OCR,IFAIL)
END

************************************************************************
SUBROUTINE COBALT(CONC,XARG,OCR)
DOUBLE PRECISION K(13),KCO(3,13),C(13),CCR(3,13),FIT,XARG
DOUBLE PRECISION X(4),Y(4),W(4),WORK1(3,4),WORK2(2,3)
DOUBLE PRECISION A(3,3),S(3),B(3),CONC,OCR,XCAP
INTEGER M,KPLUS1,NROWS,IFAIL,NPLUS1
DATA CCO(1,1),CCO(1,2),CCO(1,3)/1.975D1,2.39D1,2.87D1/,
 * CCO(1,4),CCO(1,5),CCO(1,6),CCO(1,7)/2.36D1,6.94D0,2.81D0,4.36D0/,
 * CCO(1,8),CCO(1,9),CCO(1,10)/1.89D0,1.47D0,0.0D0/,
 * CCO(1,11),CCO(1,12),CCO(1,13)/0.0D0,0.0D0,0.0D0/,
 * CCO(2,1),CCO(2,2),CCO(2,3),CCO(2,4)/1.58D1,7.87D0,2.36D0,1.78D0/,
 * CCO(2,5),CCO(2,6),CCO(2,7)/1.8D1,8.52D0,3.82D0/,
 * CCO(2,8),CCO(2,9),CCO(2,10)/6.15D0,3.92D0,0.0D0/,
 * CCO(2,11),CCO(2,12),CCO(2,13),CCO(3,1)/0.0D0,0.0D0,0.0D0,3.51D1/,
 * CCO(3,2),CCO(3,3),CCO(3,4)/4.08D1,3.59D1,4.98D1/,
 * CCO(3,5),CCO(3,6),CCO(3,7)/-1.87D1,3.59D1,2.365D1/,
 * CCO(3,8),CCO(3,9),CCO(3,10)/1.88D1,1.09D1,0.0D0/,
 * CCO(3,11),CCO(3,12),CCO(3,13),KCO(1,1)/0.0D0,0.0D0,0.0D0,1.0D2/,
 * KCO(1,2),KCO(1,3),KCO(1,4),KCO(1,5)/1.0D2,1.0D2,1.0D2,1.4D2/,
 * KCO(1,6),KCO(1,7),KCO(1,8),KCO(1,9)/2.0D2,3.1D2,4.2D2,6.0D2/,
 * KCO(1,10),KCO(1,11),KCO(1,12)/7.5D2,7.5D2,7.5D2/,
 * KCO(1,13),KCO(2,1),KCO(2,2),KCO(2,3)/7.5D2,1.0D2,1.0D2,1.0D2/,
 * KCO(2,4),KCO(2,5),KCO(2,6),KCO(2,7)/1.0D2,1.5D2,1.7D2,2.4D2/,
 * KCO(2,8),KCO(2,9),KCO(2,10)/3.286D2,4.25D2,7.5D2/,
 * KCO(2,11),KCO(2,12),KCO(2,13),KCO(3,1)/7.5D2,7.5D2,7.5D2,1.0D2/,
 * KCO(3,2),KCO(3,3),KCO(3,4),KCO(3,5)/1.0D2,1.0D2,1.0D2,1.3D2/,
 * KCO(3,6),KCO(3,7),KCO(3,8),KCO(3,9)/1.6D2,2.1D2,2.5D2,3.4D2/,
 * KCO(3,10),KCO(3,11),KCO(3,12),KCO(3,13)/7.5D2,7.5D2,7.5D2,7.5D2/
311 DATA NCAP7,IFAIL/13,0/
312 DATA X(1),X(2),X(3),X(4),Y(1)/0.0000,1.0000,2.0000,3.0000/,
313 * W(1),W(2),W(3),W(4)/1.0000,1.0000,1.0000,1.0000/
314 DATA M,KPLUS1,NROWS,NPLUS1/4,3,3,3/
315 DO 8 I = 1,3
316 DO 5 J = 1,13
317 K(J) = KCO(I,J)
318 5 C(J) = CCO(I,J)
319 CALL E02BBF(NCAP7,K,C,XARG,AT,IFAIL)
320 8 Y(I+1) = AT
321 CALL E02ADF(M,KPLUS1,NROWS,X,Y,W,WORK1,WORK2,A,S,IFAIL)
322 DO 12 I = 1,3
323 12 B(I) = A(3,I)
324 XCAP = (2.0D0*CONC-X(4))/X(4)
325 CALL E02AEF(NPLUS1,B,XCAP,DCO,IFAIL)
326 END
327 ************************************************************************
328 SUBROUTINE PHOS(X,P,Il)
329 C
330 C CALCULATES STRENGTHENING DUE TO PHOSPHORUS AT 23DEGC
331 C
332 DOUBLE PRECISION X,P
333 DATA DTAUDC/1.28D2/
334 P = DTAUDC*X
335 IF (X.GT.1.98D-1) Il = 1
336 END
337 ************************************************************************
338 SUBROUTINE RESULT(DSRES,ELSE,I2,I555)
339 DOUBLE PRECISION C(15),DAT(15),DSRES(15),ELSE(15),TTLSUM(500)
340 DOUBLE PRECISION DSB,DSC,DSN,FE,SUM1,SUM2,SYFE,T,TOTAL
341 INTEGER 12(15)
342 COMMON/TOT/TTLSUM
343 COMMON/PARMS/C,DAT,T
344 C
345 C COMMON BLOCK SHC CONNECTS TO FINAL SUBROUTINE FOR
346 C CALCULATION OF STRAIN HARDENING COEFFICIENTS
347 C
348 COMMON/SHC/TOTAL
349 WRITE(6,20)T,T-273
CALL IRON(T,SYFE)
IF (DAT(13).GT.O.ODO) CALL CARBON(DSC)
DO 10 I = 1,12
IF (DAT(I).GT.O.ODO) THEN
  CALL NAME(I)
  WRITE(6,50)DAT(I),C(I)
  IF (LLE.5 .OR. LEQ.12) WRITE(6,46)
  IF (LEQ.6) WRITE(6,47)
  IF (LEQ.8 .OR. LEQ.9) WRITE(6,47)
  IF (I2(I).EQ.1) WRITE(6,49)
  IF (T.EQ.2.96D2) THEN
    WRITE(6,60)2.0DO*DSRES(I)
    IF (LLE.5) WRITE(6,61)ELSE(I)
    IF (LEQ.2) WRITE(6,65)
  ELSE
    IF (LLE.5) THEN
      WRITE(6,51)
      WRITE(6,60)ELSE(I)
    ELSE
      WRITE(6,52)
      WRITE(6,60)2.0DO*DSRES(I)
    ENDIF
  ENDIF
ENDIF
10 CONTINUE
DSN = O.ODO
DSB = O.ODO
CALL NANDB(DSN,DSB)
SUM1 = SYFE + DSC + DSN + DSB - 2.0DO*DSRES(2) + ELSE(2)
SUM2 = SYFE + DSC + DSN + DSB
IF (T.EQ.2.96D2) TOTAL = 2.0DO*ADD(DSRES) + SUM1
IF (T.NE.2.96D2) TOTAL = ADD(ELSE) + SUM2
WRITE(6,70)TOTAL
1TLSUM(I555) = TOTAL
20 FORMAT(' AABS1.PROP:IRON',
  * /,' FOR INFO SEE AABS1.PROP:SPEC',
  * /,' FOR REFERENCES SEE AABS1.PROP:REFS',
  * /,' ALL VALUES APPLY TO NORMAL YIELD STRESS',
  * /,' TEMPERATURE =','F6.1','K','F5.1','DEGC')
389 46 FORMAT(' STRAIN RATE = 0.25E-3/S')
390 47 FORMAT(' STRAIN RATE IN RANGE 0.1E-4 TO 0.1E-2/S')
391 49 FORMAT(' ***CONCENTRATION EXTRAPOLATED***')
392 50 FORMAT(F7.4,' WT%(',F4.2,' AT%)')
393 51 FORMAT(' TEMPERATURE DEPENDENT CALCULATION')
394 52 FORMAT(' AS FOR 23DEGC')
395 60 FORMAT(' DELTA SIGMA =',F6.2,'MPA')
396 61 FORMAT(' (TEMPERATURE DEPENDENT CALCULATION: DELTA SIGMA =',F6.2,'MPA)')
397 65 FORMAT(' ***TEMPERATURE DEPENDENT VALUE IS TAKEN***')
398 70 FORMAT(/,' TOTAL =',F7.2,'MPA')
400 END
401 ************************************************************************
402 SUBROUTINE IRON(T1,FE)
403 C
404 C ESTIMATES THE EFFECT OF TEMPERATURE AND STRAIN RATE ON THE
405 C STRESS OF PURE IRON USING DATA FROM CHRISTIAN AND ALTSHULER.
406 C
407 IMPLICIT DOUBLE PRECISION (F)
408 DOUBLE PRECISION K(12),C(12),GRAD,REF,SRATE,T1,X1,X2,X3
409 INTEGER NCAP7,IFAIL,I10
410 COMMON/P ARM/SRA TE
411 DATA C(1),C(2),C(3),C(4),C(5)/6.78D1,5.83D1,6.75D1,5.0D1,4.05D1/,
412 * C(6),C(7),C(8),C(9),C(10)/2.66D1,2.4D1,2.25D1,0.0D0,0.0D0/,  
413 * C(11),C(12),K(1),K(2),K(3)/0.0D0,0.0D0,1.0D2,1.0D2,1.0D2/,  
414 * K(4),K(5),K(6),K(7),K(8)/1.0D2,1.4D2,1.9D2,2.25D2,2.6D2/,  
415 * K(9),K(10),K(11),K(12)/3.0D2,3.0D2,3.0D2,3.0D2/  
416 DATA FE296,FE300,REF/2.3D1,2.26D1,4.0D-4/  
417 DATA NCAP7,IFAIL,I10/12,O,O/  
418 IF (T1.GE.2.6D2) THEN
419 SRATE=2.5D-4
420 IF (SRATE.EQ.0.0D0) SRATE = 4.0D-4
421 ELSE
422 IF (T1.GT.1.65D2 .AND. T1.LE.1.95D2) THEN
423 IF (SRATE.EQ.0.0D0) SRATE = 4.0D-4
424 ELSE
425 IF (SRATE.EQ.0.0D0) SRATE = 5.0D-4

107
REF = 5.0D-4
110 = 1
ENDIF
ENDIF

GRAD = 2.38DO + (1.84D-3*T1)
X1 = DLOG10(REF)
X2 = DLOG10(SRATE)
X3 = (X1-X2)*GRAD
IF (T1.GE.3.0D2) THEN
FE = (FE300 - X3)*9.80665D0
ENDIF

C THIS ASSUMPTION IS BASED ON FIG. 6 OF CONRAD AND FREDRICK, WHICH
C SHOWS THERE TO BE LITTLE CHANGE IN STRENGTH WITH TEMPERATURE
C ABOVE 300K. THEIR DATA IS NOT USED BECAUSE THEIR IRON WAS NOT VERY
C PURE.

C THE 9.80665 FACTOR CONVERTS KGF.MM-2 TO MPA.

WRITE(6,810)T1,FE,SRATE
IF (T1.GT.3.0D2) WRITE(6,825)
IF (T1.GT.3.0D2 .AND. SRATE.NE.4.0D-4) WRITE(6,830)
ELSE
CALL E02BBF(NCAP7,K,C,T1,FE,IFAIL)
FE = (FE - X3)*9.80665D0
WRITE(6,810)T1,FE,SRATE
IF (T1.GT.3.0D2 .AND. SRATE.NE.4.0D-4) WRITE(6,830)
ENDIF

FORMAT(‘ UPPER YIELD STRESS OF PURE IRON AT’,F6.1,’K =’,F7.2,’MPA’
*’,
*’ STRAIN RATE =’,E9.2,’/S’)
FORMAT(‘ BUT N.B., STRAIN RATE DATA IS ONLY APPROXIMATE AT
THIS TE
*MPERATURE’)
825 FORMAT(’ ***TEMPERATURE SCALE EXTRAPOLATED***’)
SUBROUTINE KIMURA(T2,STRAT,X4)

C
C ESTIMATES THE EFFECT OF TEMPERATURE AND STRAIN RATE ON THE
YIELD
C STRESS OF PURE IRON, COMBINING DATA FROM KIMURA ET AL. WITH
RESULTS
C FROM CHRISTIAN AND ALTSHULER

DOUBLE PRECISION K(11),C(1),FE,T2,STRAT,X4
INTEGER NCAP7,IFAIL
DATA C(1),C(2),C(3),C(4),C(5)/2.0D2,1.95D2,1.78D2,8.92D1,6.21D1/, 
*C(6),C(7),C(8),C(9),C(10)/4.28D1,3.51D1,0.0D0,0.0D0,0.0D0/, 
*C(11),K(1),K(2),K(3),K(4)/0.0D0,1.5D2,1.5D2,1.5D2/, 
*C(15),K(5),K(6),K(7),K(8),K(9)/2.2D2,2.4D2,2.65D2,3.0D2,3.0D2/, 
*C(10),K(10)/3.0D2,3.0D2/
DATA NCAP7,IFAIL/11,0/
CALL E02BBF(NCAP7,K,C,TI,FE,IFAIL)
FE = FE - X4
IF (SRATE.NE.8.3D-5) WRITE(6,890)
FORMAT('ALTHOUGH C.F.: SIGMA 0.1/LYS (REF. KIMURA ET AL.):', 
*F6.2,'MPA')
END

SUBROUTINE CARBON(DC1SS)

C
C CALCULATES STRENGTHENING DUE TO CARBON AT ROOM T:
C 29.4.87: STRENGTHENING DUE TO CARBON TAKEN AS ZERO

DOUBLE PRECISION C(15),DAT(15),DC1,DC1SS,DC2,DC3,T
COMMON/PARMS/C,DAT,T
CALL NAME(13)
WRITE(6,910)DAT(13),C(13)
498 DCISS = 0.000
499 IF (DAT(13).LE.5.0D-3) WRITE(6,920)
500 DC1 = C(13)/1.0D2
501 DC1 = (6.259D2*SQRT(DC1))^1.54443D1
502 C
503 C THE 1.54443D1 FACTOR CONVERTS TONs.IN-2 TO MPA
504 C
505 WRITE(6,940)DC1
506 C
507 C ALLOWS FOR THE LOW SOLUBILITY OF C IN FE
508 C
509 WRITE(6,945)DCISS
510 IF (C(13).GT.9.694D-1) WRITE(6,950)
511 DC2 = C(13)/1.0D2
512 DC2 = (6.875D2*DSQRT(DC2))^1.54443D1
513 WRITE(6,960)DC2
514 IF (C(13).GT.1.23500) WRITE(6,950)
515 DC3 = (3.802D1*DAT(13) + 2.551D1*DAT(13)*DAT(13))*6.89476D0
516 C
517 C THE 6.89476D0 FACTOR CONVERTS 1000PSI TO MPA
518 C
519 WRITE(6,980)DC3
520 910 FORMAT(F6.3,' WT%C ,F4.2,' AT%')
521 920 FORMAT(' NOTE: ACCURATE DATA ON THE STRENGTHENING DUE TO
CARBON AT
522 * THIS','/,' CONCENTRATION IS AVAILABLE, (REFS. BAIN AND PAXTON/KIMU
523 * RA ET AL.).')
524 940 FORMAT(' N.B. HIGH NICKEL (20-30WT%) STEEL DATA /0.2PS
COMPRESSION
525 *','/,' STRENGTHENING IS ESSENTIALLY ATERMAL (REF. CHRISTIAN'),
526 *',' LATH MARTENSITE: DELTA SIGMA =','F7.2,'MPA')
527 945 FORMAT(' => STRENGTHENING DUE TO CARBON IN SOLUTION: DELTA
SIGMA =
528 *','F6.2,'MPA')
529 950 FORMAT(' ***CONCENTRATION EXTRAPOLATED***')
530 960 FORMAT(' (TWINNED MARTENSITE: DELTA SIGMA =','F7.2,'MPA')
531 980 FORMAT(' INFLUENCE OF CARBON ON YIELD STRENGTH OF STEEL
SECTIONS,'
532 *',' (REF. BAIN AND PAXTON);','F6.2,'MPA')

110
571 C
572 DOUBLE PRECISION C(15),DAT(15),CB(9),KB(9)
573 DOUBLE PRECISION BOR,DB,DBB,DN,NIT,NIT200,NIT300,PPM,T
574 INTEGER NCAP7,IFAIL
575 COMMON/PARMS/C,DAT,T
576 DATA CB(1),CB(2),CB(3),CB(4)/0.0D0,1.0D2,1.21D2,1.21D2/
577 * CB(5),CB(6),CB(7),CB(8),CB(9)/1.24D2,0.0D0,0.0D0,0.0D0/
578 * ,KB(1),KB(2),KB(3),KB(4)/0.0D0,0.0D0,0.0D0,0.0D0/
579 * KB(5),KB(6),KB(7),KB(8),KB(9)/2.5D1,1.4D2,1.4D2,1.4D2,
580 DATA BOR,NIT/3.151D4,4.344D3/
581 DATA NCAP7,IFAIL,9,0/
582 DO 88 I = 14,15
583 IF (C(I).GT.0.0D0) THEN
584 CALL NAME(I)
585 IF (I.EQ.14) THEN
586 IF (DAT(14).EQ.0.0D0) THEN
587 DN = 0.0D0
588 ELSE
589 NIT200 = 2.58 - (5.31D3*DAT(14)) + 1.455D5*DAT(14)*DAT(14)
590 NIT300 = 7.35 + (0.44D4*DAT(14)) - 0.594D5*DAT(14)*DAT(14)
591 DN = 1.0D-2*(NIT300-NIT200)*(T-2.0D2) + NIT200
592 ENDIF
593 WRITE(6,1010)DAT(14),C(I)*1.0D4,C(I),DN
594 ELSE
595 PPM = C(I)*1.0D4
596 IF (PPM.LT.1.4D2) THEN
597 CALL E02BBF(NCAP7,KB,CB,PPM,DB,IFAIL)
598 WRITE(6,1015)DAT(I5),PPM,C(I5),DB
599 ELSE
600 WRITE(6,1020)
601 ENDIF
602 DBB = DAT(15)*BOR
603 WRITE(6,1030)DBB
604 ENDIF
605 ENDIF
606 88 CONTINUE
607 1010 FORMA(F7.4," WT%","F4.0," ppm.atoms/","F6.4," AT%"),
608 */", DELTA SIGMA ="F6.2," MPA",
609 */" (APPROX.)")
DC1SS = 0.0D0
499 IF (DAT(13).LE.5.0D-3) WRITE(6,920)
500 DC1 = C(13)/1.0D2
501 DC1 = (6.259D2*SQRT(DC1)*1.54443D1
502 C
503 C THE 1.54443D1 FACTOR CONVERTS TONS.IN-2 TO MPA
504 C
505 WRITE(6,940)DC1
506 C
507 C ALLOWS FOR THE LOW SOLUBILITY OF C IN FE
508 C
509 WRITE(6,945)DC1SS
510 IF (C(13).GT.9.694D-1) WRITE(6,950)
511 DC2 = C(13)/1.0D2
512 DC2 = (6.875D2*DSQRT(DC2)*1.54443D1
513 WRITE(6,960)DC2
514 IF (C(13).GT.1.235DO) WRITE(6,950)
515 DC3 = (3.802D1*DAT(13) + 2.551D1*DAT(13)*DAT(13))*6.89476D0
516 C
517 C THE 6.89476D0 FACTOR CONVERTS 1000PSI TO MPA
518 C
519 WRITE(6,980)DC3
520 910 FORMAT(F6.3,' WT%(' ,F4.2,' AT%)')
521 920 FORMAF(' NOTE: ACCURATE DATA ON THE STRENGTHENING DUE TO
CARBON AT
522 * THIS',/,' CONCENTRATION IS AVAILABLE, (REFS. BAIN AND PAXTON/KIMU
523 *RA ET AL.).'
524 940 FORMAT(' N.B. HIGH NICKEL (20-30WT%) STEEL DATA /0.2PS
COMPRESSION
525 *',/,' STRENGTHENING IS ESSENTIALLY ATERMAL (REF. CHRISTIAN)',
526 * /,' LATH MARTENSITE: DELTA SIGMA =','F7.2,'MPA')
527 945 FORMAT(' => STRENGTHENING DUE TO CARBON IN SOLUTION: DELTA
SIGMA =
528 *','F6.2,'MPA')
529 950 FORMAT(' ***CONCENTRATION EXTRAPOLATED***')
530 960 FORMAT(' (TWINNED MARTENSITE: DELTA SIGMA =','F7.2,'MPA'))
531 980 FORMAT(' INFLUENCE OF CARBON ON YIELD STRENGTH OF STEEL
SECTIONS,'
532 *',/,' (REF. BAIN AND PAXTON):','F6.2,'MPA')
533 END
534 ************************************************************************
535 SUBROUTINE NAME(M)
536 IF (M.EQ.1) WRITE(6,31)
537 IF (M.EQ.2) WRITE(6,32)
538 IF (M.EQ.3) WRITE(6,33)
539 IF (M.EQ.4) WRITE(6,34)
540 IF (M.EQ.5) WRITE(6,35)
541 IF (M.EQ.6) WRITE(6,36)
542 IF (M.EQ.7) WRITE(6,37)
543 IF (M.EQ.8) WRITE(6,38)
544 IF (M.EQ.9) WRITE(6,39)
545 IF (M.EQ.10) WRITE(6,40)
546 IF (M.EQ.11) WRITE(6,41)
547 IF (M.EQ.12) WRITE(6,42)
548 IF (M.EQ.13) WRITE(6,43)
549 IF (M.EQ.14) WRITE(6,44)
550 IF (M.EQ.15) WRITE(6,45)
551 31 FORMAT(/, 'NICKEL')
552 32 FORMAT(/, 'MANGANESE')
553 33 FORMAT(/, 'SILICON')
554 34 FORMAT(/, 'CHROMIUM')
555 35 FORMAT(/, 'COBALT')
556 36 FORMAT(/, 'VANADIUM')
557 37 FORMAT(/, 'TITANIUM')
558 38 FORMAT(/, 'MOLYBDENUM')
559 39 FORMAT(/, 'ALUMINIUM')
560 40 FORMAT(/, 'NIOBium')
561 41 FORMAT(/, 'DUMMY')
562 42 FORMAT(/, 'PHOSPHORUS')
563 43 FORMAT(/, 'CARBON')
564 44 FORMAT(/, 'NITROGEN')
565 45 FORMAT(/, 'BORON')
566 END
567 ************************************************************************
568 SUBROUTINE NANDB(DN, DBB)
569 C
570 C CALCULATES STRENGTHENING DUE TO NITROGEN AND BORON AT ROOM
C

DOUBLE PRECISION C(15),DAT(15),CB(9),KB(9)
DOUBLE PRECISION BOR,DB,DBB,DN,NIT,NIT200,NIT300,PPM,T
INTEGER NCAP7,IFAIL
COMMON/PARMS/C,DAT,T
DATA CB(1),CB(2),CB(3),CB(4)/0.0D0,1.0D2,1.21D2,1.21D2/,
CB(5),CB(6),CB(7),CB(8),CB(9)/1.24D2,0.0D0,0.0D0,0.0D0/,
KB(1),KB(2),KB(3),KB(4)/0.0D0,0.0D0,0.0D0,0.0D0/,
KB(5),KB(6),KB(7),KB(8),KB(9)/2.5D1,1.4D2,1.4D2,1.4D2/,
DATA BOR,NIT/3.151D4,4.344D31
DATA NCAP7,IFAIL/1,0/
DO 88 I = 14,15
IF (C(I).GT.0.0D0) THEN
   CALL NAME(I)
   IF (I.EQ.14) THEN
      IF (DAT(14).EQ.0.0D0) THEN
         DN = 0.0D0
      ELSE
         NIT200 = 2.58 - (5.31D3*DAT(14)) + 1.455D5*DAT(14)*DAT(14)
         NIT300 = 7.35 + (0.44D4*DAT(14)) - 0.594D5*DAT(14)*DAT(14)
         DN = 1.0D-2*(NIT300-NIT200)*(T-2.0D2) + NIT200
      ENDIF
      WRITE(6,1010)DAT(14),C(14)*1.0D4,C(14),DN
   ELSE
      PPM = C(15)*1.0D4
      IF (PPM.LT.1.4D2) THEN
         CALL E02BBF(NCAP7,KB,CB,PPM,DB,IFAIL)
         WRITE(6,1015)DAT(15),PPM,C(15),DB
      ELSE
         WRITE(6,1020)
      ENDIF
      DBB = DAT(15)*BOR
      WRITE(6,1030)DBB
   ENDIF
   88 CONTINUE

WRITE(6,1010)DAT(14),C(14)*1.0D4,C(14),DN
ELSIF (C(15)*1.0D4)
WRITE(6,1015)DAT(15),PPM,C(15),DB
WRITE(6,1020)
ENDIF
WRITE(6,1030)DBB
ENDIF
88 CONTINUE

1010 FORMAT(F7.4,' WT%(',F4.0,' ppm.atoms/',F6.4,' AT%)',
         I,' DELTA SIGMA =',F6.2,'MPA',
         I,' (APPROX.)')
610 1015 FORMAT(F7.4,' Wt%',' F4.0,' ppm',' F6.4,' AT%'),
611 * ',', 'DERIVED FROM STEEL DATA /STRAIN RATE NOT GIVEN',
612 * ',', 'ROOM TEMPERATURE',,
613 * ',', 'DELTA SIGMA =',' F6.2,'MPA')
614 1020 FORMAT(' ***MAX. CONCENTRATION IS 0.0027WT%(140PPM), BUT...')
615 1030 FORMAT(' C.F.: 0.2PS (REF. IRVINE AND PICKERING);','F7.2,'MPA')
616 END
617 ************************************************************************
618 SUBROUTINE NCALC (YLDSTR, VAL, VAC)
619 IMPLICIT REAL*8 (A-H,O-$)
620 COMMON/SHC/SUM
621 DATA ENM/1.0D-4/
622 VAL = VAL/1.0D2
623 VAC = VAC/1.0D2
624 VW = 1.0 - VAL - VAC
625 SY = VAL*124.4D0*((0.002DO)**0.644DO)
626 SY = SY
627 SY = SY + VW*478.1DO*((0.002DO)**0.0812DO)
628 SUTS = VAL*124.4D0*((0.644DO)**0.644DO)
629 SUTS = SUTS
630 SUTS = SUTS + VAC*498.5DO*((0.0812DO)**0.0812DO)
631 C
632 C ITERATION TO FIND STRAIN HARDENING COEFFICIENT
633 C
634 SY = SY + SUM
635 SUTS = SUTS + SUM
636 4 CONTINUE
637 ARGUM = (SY/SUTS) - ((0.002DO/ENM)**ENM)
638 ENM = ENM + 1.D-6
639 IF (ARGUM.LT.0.00001DO) GOTO 4
640 YLDSTR = YLDSTR*(0.1D0**ENM)
641 RETURN
642 END
643%
644 FILE .DATA TO .OUT:ONE
645 FILE .OUT:TWO TO &A
646 COMMENT DATA IS IN .OUT:ONE
647 COMMENT RESULTS ARE IN .OUT:TWO
648 COMMENT COPY FOR EDITING IS IN &A
APPENDIX 5: STRAIN-HARDENING COEFFICIENTS PROGRAM

FrVSCLR PROGRAM=%H% DATA=.NREG:DATA NAG OUTPUT=&OUT


MINIMIZATION PROGRAM FOR EVALUATION OF STRAIN-HARDENING COEFFICIENTS

KEY: X(3) = KAL = K alpha
X(2) = KW = K W
X(1) = KAC = K a
X(4) = NAL = n alpha
X(5) = NW = n W
X(6) = NAC = n a

IMPLICIT REAL*8(A-H,K,N-$)

DOUBLE PRECISION SIGMY(35), SIGUTS(35), VAL(35), VW(35), VAC(35)

DOUBLE PRECISION FVEC(6), WA(100), X(6)

DOUBLE PRECISION DIAG(8), FJAC(7,7), R(30), QTF(6), W(6,5)

COMMON/AABS I/SIGMY,SIGUTS,VAL,VW,VAC

EXTERNAL FCN

DATA MAXFEV, ML, MU, MODE, MPRINT/ 1500, 5, 5, 1, 1/ 
DATA XTOL, EPSFCN, FACTOR / 1.0D-7, 0.0D0, 100.0D0/ 
DATA LDFJAC, LR, IFAIL/ 7, 30, 0/ 

DO 4 I = 1,35
READ(5,*)SIGMY(I), SIGUTS(I), VAL(I), VAC(I)

VW(I) = 1.0D0 - VAL(I) - VAC(I)
CALL C05NCF(FCN,6,X,FVEC,XTOL,MAXFEV,ML,MU,MPRINT,MFEV,FJAC,LDFJAC,
R,LR,QTF,W,IFAIL)

FNORM=F05ABF(FVEC,6)
WRITE(6,55)X(3),X(2),X(1),X(4),X(5),X(6)
STOP

FORMAT(' KAL =',F11.6/, KW =',F11.6/, 
KAC =',F11.6/, NAL =',F9.6/, 
NW =',F9.6/, NAC =',F9.6)

END

SUBROUTINE FCN(J,X,EQN,IFLAG)

IMPLICIT REAL*8(A-H,K,N-$)

DOUBLE PRECISION SIGMY(35), SIGUTS(35), VAL(35), VW(35), VAC(35)
38 DOUBLE PRECISION EQN(6),X(6)
39 COMMON/AABS1/SIGMY,SIGUTS,VAL,VW,VAC
40 J = 6
41 IF (J1.EQ.0) THEN
42 C
43 C INITIAL GUESS VALUES
44 C
45 X(3) = 202.000
46 X(2) = 504.000
47 X(1) = 526.000
48 X(4) = 0.59500
49 X(5) = 0.07200
50 X(6) = 0.09400
51 ENDIF
52 J1 = 1
53 WRITE(6,77)X(3),X(2),X(1),X(4),X(5),X(6)
54 SUMMY = ADD(SIGMY)
55 SUMVAL = ADD(VAL)
56 SUMVW = ADD(VW)
57 SUMVAC = ADD(VAC)
58 SUMUTS = ADD(SIGUTS)
59 ARGY = SUMMY - SUMVAL*X(3)*((0.00200)**X(4))
60 ARGY = ARGY - SUMVW*X(2)*((0.00200)**X(5))
61 ARGY = ARGY - SUMVAC*X(1)*((0.00200)**X(6))
62 ARGUTS = SUMUTS - SUMVAL*X(3)*(X(4)**X(4))
63 ARGUTS = ARGUTS - SUMVW*X(2)*(X(5)**X(5))
64 ARGUTS = ARGUTS - SUMVAC*X(1)*(X(6)**X(6))
65 EQN(1) = ARGY*SUMVAL*((0.00200)**X(4))
66 EQN(1) = EQN(1) + ARGUTS*SUMVAL*(X(4)**X(4))
67 EQN(2) = ARGY*SUMVW*((0.00200)**X(5))
68 EQN(2) = EQN(2) + ARGUTS*SUMVW*(X(5)**X(5))
69 EQN(3) = ARGY*SUMVAC*((0.00200)**X(6))
70 EQN(3) = EQN(3) + ARGUTS*SUMVAC*(X(6)**X(6))
71 EQN(4) = ARGY*SUMVAL*X(3)*(-6.214600)*((0.00200)**X(4))
72 E4 = ARGUTS*SUMVAL*X(3)*(X(4)**X(4))*(1.000+DLOG(X(4)))
73 EQN(4) = EQN(4) + E4
74 EQN(5) = ARGY*SUMVW*X(2)*(-6.214600)*((0.00200)**X(5))
75 EQN5 = ARGUTS*SUMVW*X(2)*(X(5)**X(5))*(1.000+DLOG(X(5)))
76 EQN(5) = EQN(5) + E5

115
77 EQN(6) = ARGY*SUMVAC*X(1)*(-6.2146D0)*((0.002D0)**X(6))
78 EQN6 = ARGUTS*SUMVAC*X(1)*(X(6)**X(6))*(1.0D0+DLOG(X(6)))
79 EQN(6) = EQN(6) + E6
80 WRITE(6,88) EQN(1),EQN(2),EQN(3),EQN(4),EQN(5),EQN(6)
81 RETURN
82 77 FORMAT(' KAL =',F11.6,',' KW =',F11.6, ',
83 & KAC =',F11.6,',' NAL =',F9.6, ',
84 & NW =',F9.6,',' NAC =',F9.6)
85 88 FORMAT(' EQN1 =',E12.5,',' EQN2 =',E12.5, ',
86 & EQN3 =',E12.5,',' EQN4 =',E12.5, ',
87 & EQN5 =',E12.5,',' EQN6 =',E12.5)
88 END
89
90 DOUBLE PRECISION FUNCTION ADD(Y)
91 DOUBLE PRECISION Y(35)
92 ADD = 0.0D0
93 DO 4 I = 1,35
94 4 ADD = ADD + Y(I)
95 RETURN
96 END
97 %
APPENDIX 6: HETEROGENEITY PROGRAM

1 FTVSCLR PROGRAM=%H% DATA=.DATA OUTPUT=&A
2 C CONCURRENT PROGRAM TO CALCULATE SCATTER AND HETEROGENEITY
3 C OF WELD METALS (TREATED AS A THREE PHASE MICROSTRUCTURE)
5 READ(5,*)N,A,B
6 C READ NO. OF SETS OF DATA, AND
7 C VOLUME FRACTIONS OF TWO OF THE PHASES
8 WRITE(6,5)N
9 DO 4 I = 1,N
10 READ(5,*)T,E
11 C READ TESTING TEMPERATURES (IN DEGREES CELSIUS)
12 C AND CHARPY ENERGIES (IN JOULES)
13 4 WRITE(6,10)T,E
14 C OUTPUT IS IN A FORMAT SUITABLE FOR GLIM
15 C (GENERALISED LINEAR INTERACTIVE MODELLING PACKAGE)
16 WRITE(6,15)
17 STOP
18 5 FORMAT(‘$ units’,I3,’$ data temp e $ read’)
19 10 FORMAT(2F8.2)
20 15 FORMAT(‘$ ,/’)
21 &’$ plot e temp $ ’/,
22 &’$ calc y=\log(e/(280-e))$ plot y temp $ ’/,
23 C THE NUMBER 280 IS THE UPPER SHELF ENERGY
24 C AND SHOULD BE ALTERED ACCORDINGLY
25 &’$ yvar y $ fit $ dis e $ ’/,
26 &’$ fit + temp $ dis e r $ plot %fv temp $ ’/,
27 &’$ end’/,
28 &’$ stop’)
29 END
30 %
31 !
32 GLIM PROGRAM=&A OUTPUT=&B
33 ! THIS PROGRAM CALCULATES THE MICROSTRUCTURAL
34 ! HETEROGENEITY OF THE THREE PHASE MICROSTRUCTURE
35 FTVSCLR %H% DATA=.DATA OUTPUT=&C
36 DOUBLE PRECISION B,C,D,HOMOG
37 READ(5,*)IB,C
38 B = B/1.0D2

117
39 \( C = \frac{C}{1.0D2} \)
40 \( D = 1.0D0 - B - C \)
41 WRITE(6,45)B,C,D
42 HOMOG = 1.0D0 - B - C
43 HOMOG = HOMOG*(DLOG(HOMOG))
44 HOMOG = HOMOG + B*(DLOG(B))
45 HOMOG = HOMOG + C*(DLOG(C))
46 HOMOG = - HOMOG
47 WRITE(6,55)HOMOG
48 STOP
49 45 FORMAT(' VOLUME FRACTIONS :',F8.4,' :',F8.4,' :',F8.4)
50 55 FORMAT(' HETEROGENEITY =',F11.4,';
51 & WHERE 0 = HOMOGENEOUS',/,
52 & AND 1.0986 = HETEROGENEOUS')
53 END
54 %


