QUANTITATIVE ANALYSIS OF TEXTURE DATA

by

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PREFACE

This dissertation is an account of work carried out in the Department of Metallurgy, University of Cambridge, from October 1967 to October 1970. The work is original, except where otherwise acknowledged, and has not been submitted, either in whole or in part, for a degree at this or any other university.

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INTRODUCTION

Each grain in a polycrystalline aggregate normally has a crystallographic orientation different from that of its neighbours. Considered as a whole, the orientations of all grains may be randomly distributed with respect to some selected frame of reference, or they may tend to cluster, to a greater or lesser degree, about some particular orientation or orientations. Any aggregate characterized by the latter condition is said to have preferred orientation, or texture, which may be defined as a condition in which the distribution of crystal orientations is non-random. Such a condition may be brought about by many processes, including casting, deformation, and heat treatment.

The importance of texture lies in the effect, often very marked, which it has on the macroscopic properties of materials. Given that most single crystals are anisotropic, it follows that, in general, an aggregate having preferred orientation will have directional properties also. Such properties may or may not be desirable, depending upon the use to which the material is put.

Textures have been studied for many years, with the aim both of understanding the development of preferred orientation, and of correlating texture with material properties. Conventional texture data, as determined by X-ray measurements, do not give a direct and unambiguous representation of the texture of a specimen, and have failed to resolve many outstanding problems associated with the development and properties of preferred orientations. Recently, however, suitable procedures have become available for the analysis of X-ray data, although because of
their complexity they have not yet become standard practice.

This work sets out to apply a quantitative analysis of texture data to certain problems in the field of texture research which have not been resolved by conventional methods, in order to assess whether any additional information or understanding is forthcoming. The dissertation is divided into three parts. Part I comprises Chapters 1, 2, and 3, and describes the experimental and analytical methods used in the course of the work. Part II, comprising Chapters 4, 5, and 6, describes an investigation of the development of rolling textures in copper and α-brass, and a simulation of the texture development based on possible deformation mechanisms. Part III, contained in Chapters 7, 8, and 9, describes the correlation of texture with anisotropy in cubic metals, with particular reference to elastic and plastic anisotropy in cold rolled sheets of copper and α-brass. A summary of the work, and suggestions for future research which could improve the understanding of textured materials, are given in Chapter 10.
PART I

EXPERIMENTAL AND ANALYTICAL PROCEDURE
1.1 Introduction

In order to describe completely the orientation of a crystal in a polycrystalline sample three independent parameters are required. For example, the orientation of a particular crystal direction with respect to arbitrary sample axes may be described by two parameters. A third parameter is required to specify the rotational degree of freedom about this axis. It is customary to characterize the orientation of a crystal in a rolled sheet by specification of those crystal planes, \{hkl\}, which lie in the plane of the sheet, and those crystallographic directions, <uvw>, which coincide with the rolling direction of the sheet. Alternatively a matrix of direction cosines describing the relation between the crystal axes and the sample axes may be given. In both of these cases, however, only three parameters are independent. It is not practical to specify the orientation of every crystal in a polycrystalline sample but a useful description of the texture of a material can be made by specifying the relative frequencies with which crystallites occur in the various orientations.

Let any three independent parameters describing a crystallite orientation be \(\alpha, \beta,\) and \(\gamma\). Then the probability, \(p\), of a crystal having an orientation in the range \(d\alpha, d\beta, d\gamma\), is:

\[
p = w(\alpha, \beta, \gamma) J d\alpha d\beta d\gamma \quad (1.1)
\]

where \(J\) is the Jacobian

\[
\int \int \int w(\alpha, \beta, \gamma) J d\alpha d\beta d\gamma = 1
\]
The function \( w(\alpha, \beta, \delta) \) describes the orientation probability distribution of the crystallites.

It has not yet proved possible to make a direct measurement of this function for a polycrystalline sample. Consequently many indirect methods have been used to obtain and present texture data. The most common of them are reviewed in this chapter.

1.2 Measurement of Textures

1.2.1 X-Ray Methods.

The most common method of determining textures in polycrystalline samples is by X-ray diffraction. These techniques may employ either grain by grain orientation determination \([1,2,3]\), or variations of the powder diffraction method \([1,2,3,4]\). The latter methods are useful over a wide range of grain sizes when suitable integration and scanning mechanisms are incorporated into the diffractometer. Early photographic methods are described by Barrett \([1]\), but these have been largely superseded by the more quantitative diffractometer techniques. More recently, automatic scanning texture diffractometers have been commercially available.

Two geometries of sheet specimen mounting relative to the incident and diffracted beams are conventionally used, so that the specimen is arranged for measurement of the transmitted \([5]\) or reflected \([6]\) beam for one Bragg reflection. Neither method gives complete sampling of all orientations of the reflecting plane normal. Complete coverage is achieved when data from both methods are matched and superimposed \([3]\).
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Several variations of specimen geometry have been proposed to provide complete coverage in reflection with one specimen. These include sectioned composite specimens [7,8], spherical specimens [9] and cylindrical specimens [10]. Bunge and Haessner [11] have shown that the use of a spherical specimen results in lower systematic errors than found in measurements made by the combined transmission and reflection method. However, many workers are attracted by the simplicity of the straightforward reflection method and are willing to forgo complete pole figure data to this end.

All of the above methods measure the intensity of a particular Bragg reflection as a function of specimen orientation, and the results are presented as pole figures (see Section 1.3). An alternative method which is especially useful if the material exhibits axial symmetry is to compare the intensities of reflections from a number of crystallographic planes, for a fixed specimen orientation. These data are plotted as an inverse pole figure (see Section 1.3). The method was used by Harris [12], corrected firstly by Mueller et al. [13] and more recently by Horta et al.[14]. The method requires the diffracted intensities to be measured of \{hkl\} planes parallel to a reference plane in the specimen. These intensities are then divided by the corresponding intensity from a specimen with a random distribution of crystallite orientations. Since only a number of discrete reflections are used, the intensity ratios need normalizing [13,14]. This method may be used for materials not exhibiting axial symmetry, but extreme care must be taken in their interpretation since there is not necessarily any correlation between the inverse pole figures for different sample directions [13].

A disadvantage of X-ray methods is that information is only obtained about either the orientation of crystal plane normals with
respect to the sample, or the orientation of a given direction in the sample with respect to the crystal axes. In both cases only two parameters are specified, rather than the three required to specify fully the relationship between the crystal axes and the sample axes. To overcome this and present a full description of texture the information from several normal or inverse pole figures must be correlated.

1.2.2 Other Diffraction Methods

Although most texture studies have involved X-ray diffraction, some work has been done with electron [11,15,16] and neutron [17] diffraction. Perlwitz et al. [15] and Bunge and Haessner[11] used selected area electron diffraction to study textures in copper alloys. This method gives the orientation of individual crystallites, and large numbers must be examined to give a picture of the overall texture. The method gives a three dimensional representation of texture in that the orientation of each crystallite is uniquely determined. Only Bunge and Haessner, however, took advantage of this, and the other workers presented their results after the elimination of one dimension. The method is tedious and the number of crystallites sampled is small (e.g. 560 [11]). The results are, therefore, subject to statistical fluctuations. Bunge and Haessner compared the results that they obtained from electron diffraction with those obtained by X-ray diffraction and concluded that any differences were due to the smaller volume of material sampled by the electron diffraction experiments.

Neutron diffraction has been used by Bunge and Tobisch [17] to measure the texture of 90 percent cold rolled copper. Neutron diffraction methods, although not suitable for all materials [3] have the advantage of good penetration and low background radiation, but
require high energy neutron sources which are not readily available. The results of Bunge and Tobisch show that very accurate results may be obtained by this method.

1.2.3 Elastic Anisotropy

Elastic modulus, being a fourth rank tensor property, is in general anisotropic in all crystal classes. The experimentally determined elastic anisotropy may thus be used to characterize the texture of a sample. Early work using the variation of Young's modulus in the rolling plane of sheet specimens of copper was performed by Weerts [18]. It was shown that, of eight f.c.c. metals examined, copper showed the greatest elastic anisotropy and has been used for most subsequent work. Weerts found poor correlation between the experimental variation of Young's modulus in 96 percent cold reduced copper, and that expected for the commonly expressed ideal orientation \{110\}<112>. Better correlation was found between the experimental and predicted curves for recrystallized copper sheet exhibiting sharp cube texture.

This method has been used recently to supplement pole figure data in assigning ideal orientations by Alers and Liu [19] for f.c.c. metals and by Hoddinott and Davies [20] for b.c.c. metals. More recently Stickels and Mould [21] have attempted to find an empirical relation linking the planar anisotropy of Young's modulus with the anisotropy of plastic strain ratio in low carbon steel sheets.

Pursey and Cox [22] have shown that the variation of elastic modulus with orientation in cubic crystals may be described completely by a fourth order spherical harmonic. The implication of this, as pointed out by Bunge and Roberts [23] is that only three independent parameters (in the form of coefficients of a spherical harmonic
expansion of the orientation distribution) may be obtained by elastic modulus measurements, and that completely different textures which agree in the values of their fourth order coefficients lead to exactly the same elastic properties. Furthermore, there is uncertainty in the averaging procedures usually adopted, those due to Voigt [24], Reuss [25], and Hill [26]. To date it has not been possible to apply the exact theories of polycrystalline elasticity, such as those due to Kroner [27] and Hill [28], to textured material. Elastic modulus measurements are, therefore, best used to complement more powerful methods.

1.2.4 Magnetic Anisotropy

Single crystals of most ferromagnetic materials exhibit magnetic anisotropy, which in general leads to anisotropy in textured aggregates. Measurements of magnetic anisotropy are relatively easy and have been used to characterize texture [29,30]. The method is based on the variation of the magnetic domain energy with the position of the magnetization vector in the crystal. Following Akulov [29] for cubic crystals:

\[
E = K_0 + K_1 \varphi_1 + K_2 \varphi_2 + \ldots \quad (1.2)
\]

where \( \varphi_1 = l_1^2 l_2^2 + l_2^2 l_3^2 + l_3^2 l_1^2 \)

\( \varphi_2 = l_1^2 l_2^2 l_3^2 \)

\( E \) = domain energy

\( l_1 \) = direction cosines of magnetization vector relative to crystal axes \( x_i \)

\( K_n \) = nth anisotropy constant

If a flat specimen is placed in a magnetic field parallel to its surface, a torque, \( T \), is developed due to the magnetic anisotropy,
where:

\[ T = \frac{\partial E}{\partial \alpha} \]

and \( \alpha \) is the angle between the field and the preferred direction in the plane. By measuring the torque at various angles to the applied field and comparing the results obtained with single and polycrystalline samples, an estimate of the texture is obtained.

In practice the only important anisotropy constants are \( K_0 \), \( K_1 \), and \( K_2 \). \( K_0 \) is the orientation independent component, and the functions \( \Phi_1 \) and \( \Phi_2 \) in equation (1.2) correspond to fourth and sixth order cubic spherical harmonics. The same drawbacks therefore apply to this method as to the measurement of texture parameters by elastic anisotropy and it is best used to supplement other texture data or in cases where the magnetic properties are of prime importance.

1.3 Representation of Textures

1.3.1 Ideal Orientations

The most concise description of the texture of a sample is a statement of the indices of the crystal planes or directions preferentially aligned with the principal axes of the specimen. For rolled sheet specimens it is customary to define the crystal plane parallel to the rolling plane and the crystal direction parallel to the rolling direction. While this method gives a satisfactory description of sharp textures such as the \( \{001\} \langle 100 \rangle \) texture found in recrystallized copper sheets [4], it is inadequate to describe the complex textures found in many cold worked metals. Evidence of this is seen in the many different descriptions of the texture of cold rolled copper [4].
1.3.2 Pole Figures

A pole figure is a stereographic projection which shows the variation in pole density with pole orientation for a selected set of crystal planes [32]. Early workers described the pole density in arbitrary units, but it is now customary to normalize the pole figure so that a specimen exhibiting uniform pole density would be assigned a pole density of unity for all orientations [4]. This is achieved either by comparing the pole figures obtained from a textured specimen with those obtained under identical conditions from a standard texture-free sample of the same material, or by setting the integrated pole density over the whole reference sphere to $4\pi$. Grewen et al. [33] consider that the latter method is the more satisfactory.

Pole figures are most frequently measured by X-ray methods [1,2,3,4]. The manual plotting of the data is quite tedious and methods have been described for the automatic plotting of pole figures [34] and data processing by computer [35,36].

The \{hkl\} pole figure is clearly related to the volume fraction of crystallites whose (hkl) plane normal $n$ coincides with a direction $s$ in the specimen. If we let the parameters $\alpha, \beta$ of equation (1.1) describe the orientation of $n$ with respect to the specimen, then the function describing the distribution of \{hkl\} poles is:

$$q_n(s) = q_n(\alpha, \beta) = \int_{\text{all } \gamma} w(\alpha, \beta, \gamma) \, d\gamma$$  \hspace{1cm} (1.3)

where $q_n(s)ds$ is the volume fraction of crystallites having their $n$ direction in the range $ds$.

Combining equations (1.1) and (1.3)
\[ \int_{\text{all } \alpha, \beta}^{} q_n(\alpha, \beta) \, J \, d\alpha \, d\beta = 1 \]

Setting \( q'_n(s) = 4\pi q_n(s) \)

\( q'_n(s) \) represents the pole figure as conventionally presented.

### 1.3.3 Inverse Pole Figures

An inverse pole figure represents the density distribution of a principal direction in a polycrystalline sample with respect to the crystal axes. The data are usually plotted in stereographic projection in the symmetry triangle of the appropriate crystal system. The data are most frequently obtained at discrete positions in the inverse pole figure by measuring the ratio of X-ray intensities from a textured and from a random sample for various Bragg reflections, due allowance being made for the small number of data points considered and for their non uniform distribution in the symmetry triangle \([13, 14]\).

More complete methods of obtaining inverse pole figures from X-ray data have been proposed. Jetter et al. \([37]\) demonstrated an iterative method to relate the distribution of various \(\{hkl\}\) reflections in the sample with inverse pole figures, and Mitchell and Rowland \([38]\) and Williams \([39]\) have given analytical techniques.

Wiglin \([40]\), Bunge \([41]\), and Roe and Krigbaum \([42]\) have all proposed the expansion of the pole density distribution and of the axis density distribution in series of spherical harmonics. The 'inversion' then consists of finding the relation between the sets of coefficients of the two expansions. These methods, although differing in detail, are equivalent in principle.

For samples exhibiting axial symmetry a single inverse pole
figure describes the texture uniquely. Jetter et al. [37] and Mitchell and Rowland [38] have proposed the use of two or three inverse pole figures to represent rolling textures. However, it has been shown [13,43] that such a representation contains less information than a set of conventional pole figures, and that the apparent ease of interpretation of inverse pole figures may be misleading as there is not necessarily any correlation between them.

1.3.4 Three Dimensional Methods

It has not yet proved possible to make a direct measurement of the texture of a polycrystalline sample as a statistical function of the three parameters required to specify completely the orientation of a crystallite. It has become obvious, however, that such a function is needed in order adequately to understand both the mechanisms of texture development and the properties of textured materials. There are essentially two methods of obtaining a three dimensional orientation distribution function.

Firstly, one may measure the orientation of as large a number of crystallites as is practicable, and determine the relative frequency of occurrence of specific orientations. In order to do this the method of measurement must sample a volume smaller than the crystallite size. For most metal samples only electron diffraction techniques are suitable [15,16].

In the second method conventional texture data, in the form of pole figures or inverse pole figures, are measured. These specify two of the three orientation parameters and the volume fraction of crystallites possessing these parameters represents the integral of the orientation density taken over all values of the third parameter (see equation
A suitable mathematical procedure is then required in order to calculate the three-dimensional function from these values. Two different methods have been proposed:

(i) An analytical method due to Roe [44] and Bunge [45], and
(ii) An iterative method due to Williams [46].

Both Roe and Bunge have chosen the Euler angles (see [47]) as parameters with which to specify the orientation of a crystallite with respect to the sample axes. Unfortunately there are two different definitions of these angles common in the literature [47] and Roe and Bunge have chosen different conventions (Fig. 1.1). The angles \((\psi, \theta, \phi)\) used by Roe are related to the \((\varphi_1, \varphi_2, \gamma)\) used by Bunge in the following way:

\[
\begin{align*}
\psi &= \varphi_1 - \pi/2 \\
\theta &= \phi \\
\phi &= \varphi_2 + \pi/2
\end{align*}
\]

The convention adopted by Roe is that used by the majority of English mathematical texts [47], as is his notation for the subsequent calculation. Since the two methods, although differing in detail, are equivalent in principle only Roe's method will be described.

Substituting the angles \(\psi, \xi (= \cos \theta), \) and \(\phi\) in equation (1.1) we obtain,

\[
p = w(\psi, \xi, \phi) \, d\psi \, d\xi \, d\phi
\]

and

\[
\iiint w(\psi, \xi, \phi) \, d\xi \, d\psi \, d\phi = 1
\]

The experimentally observed data consist of a set of functions \(q_i(\xi, \eta)\)
Figure 1.1. Stereographic projection illustrating the Euler angles relating the crystal axes with the specimen sheet normal direction (ND) and rolling direction (RD).

a) As defined by Roe.

b) As defined by Bunge.
describing the orientation distribution of the plane normals of the ith crystal plane with respect to the sample (where $\cos^{-1} \theta$ is the polar angle, and $\eta$ the azimuthal angle). These data are expanded into a series of spherical harmonics.

$$q_i(\theta, \eta) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Q_{lm} F_{l}^{m}(\theta) e^{-im\eta}$$

As the spherical harmonics form an orthogonal set the coefficients $Q_{lm}$ may be obtained easily from the experimental data [44]. The crystallite orientation distribution function can be expanded similarly to give:

$$w(\psi, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} W_{lmn} Z_{lmn}(\theta) e^{im\psi - in\phi}$$

where $Z_{lmn}$ is a generalization of the associated Legendre function. By determining the relations between the coefficients of the two series it is possible to derive the function $w(\psi, \theta, \phi)$. The effect of crystal and specimen symmetry is to restrict the possible values of $Q_{lm}$ and $W_{lmn}$ [44,48]. This results in considerably less computation than equation (1.4) and equation (1.5) would suggest.

In practice it is necessary to truncate the series expansion after a finite number of terms. The series appears to converge fairly rapidly [11,49] and this truncation is not a great drawback. Roe [44] has given methods of estimating the truncation error.

The method of Williams [46] for obtaining a 'biaxial pole figure' is to consider the distribution function divided into a finite number of elements and to determine the effect of each element on the various pole figures. By successive iterations, each time minimising the difference between the observed and predicted pole figures, an estimate
of the three dimensional function is obtained. Williams found that nine iterations were adequate to give biaxial pole figures for cold rolled copper, aluminium, and brass.

Williams has used the angles $\alpha$, $\rho$, and $\beta$ (Williams' notation) as the parameters specifying the crystallite orientation. These are related to the Euler angles as used by Roe in the following way:

$$\begin{align*}
\alpha &= \phi \\
\rho &= \theta \\
\beta &= \psi + \tan^{-1}(\tan \phi \cos \theta)
\end{align*}$$

In presenting his results Williams has represented $\alpha$ and $\rho$ in stereographic projection, with a linear $\beta$ axis perpendicular to the projection plane. This representation results in simpler symmetries than found when using Euler's angles plotted on a Cartesian coordinate system [46]. This is not a great advantage, and most of the three dimensional analyses that have been reported in the literature have had the results presented as a series of charts with the angular coordinates plotted on rectangular Cartesian axes (see e.g. [11, 17, 23, 49]).

A large amount of computation is required with both the spherical harmonic method and the iterative method. Access to an electronic computer is essential if the analysis is to be performed in a reasonable period of time (Morris [49] has reported that a complete mapping of the function requires typically 2 hours of computation time with an IBM 360 computer). Because of this it seems that three dimensional texture analysis is best applied to problems where conventional methods have proved unsatisfactory.
2.1 Introduction

In this chapter the experimental techniques used in the preparation and testing of specimens are described. Many of these techniques are standard laboratory practice, and consequently description of these will be kept to a minimum.

2.2 Materials

All of the experimental work described in this dissertation was performed on copper and copper-zinc alloys. Three different compositions were used containing 0, 10, and 30 percent zinc respectively. The metal used was of commercial purity, the principal impurity being lead (~0.5 percent maximum). As supplied the material was in sheets 3.2 mm (0.125 in.) thick, having followed a typical production schedule of hot rolling to within 50 percent of size, followed by cold rolling with an intermediate and final anneal at 600°C. As a consequence of this a certain amount of initial texture was present (see Chapter 5). The initial grain size was found to be 0.03 mm in both the copper and the Cu - 10 percent Zn, and 0.04 mm in the Cu - 30 percent Zn.

2.3 Cold Rolling Procedure

The mill used for cold rolling was a W.H.A. Robertson two high rolling mill, with 8 inch diameter rolls, 8 inches in width. Guides were used to ensure constancy of rolling direction. Rolling was performed on
specimens 4 inches wide, with an initial length of 9 inches. The rolling schedule followed was: 0.020 in. (0.5 mm) per pass until within 0.020 in. of size, 0.005 in. (0.125 mm) per pass until within 0.005 in. of size, 0.001 in. (0.025 mm) per pass to size. The material was reversed between passes, and lubricated with Shell 'Vitrea 79' mineral oil to reduce frictional effects.

2.4 X-ray Procedures

2.4.1 Specimen Preparation

A composite sampling technique was used to prepare specimens for pole figure measurement. The method used was based on that described by Leber [50] and Elias and Heckler [8]. This method enables a complete quadrant of a pole figure to be obtained with one reflection specimen. Coupons were cut from the rolled sheet at 45° from the rolling direction. The coupons were cleaned by immersing them in a chemical polishing solution, which also served to remove the surface material which had been in contact with the rolls (about 0.02 mm was removed). The polishing solution used was:

\[
\text{HNO}_3 \quad 33 \text{ percent} \\
\text{H}_3\text{PO}_4 \quad 33 \text{ percent} \\
\text{H}_2\text{O} \quad \text{balance}
\]

and was used at room temperature. The coupons were then bonded together with Araldite epoxy resin to form a block. Coupons corresponding to each of the four quadrants were mixed [51] as an average pole figure for the four quadrants was required. A specimen was cut from the block at an angle of 54.7° from the plane of the sheets, either by spark machine, or with an abrasive cut off wheel.
In order to remove deformed metal from the cut surfaces, the specimens were mechanically polished on successive grades of abrasive paper, and finally on a 6\(\mu\)m diamond polishing wheel. They were then chemically polished to remove the remainder of the worked material. The thickness of material removed by chemical polishing was about 0.05 mm.

Microscopic examination of the completed specimen revealed that the thickness of the adhesive layer between coupons was typically 0.01 mm thick.

2.4.2 Preparation of Randomly Oriented Specimens

Random specimens of the materials used were required to establish the defocussing characteristics of the texture goniometer with the settings as used for analysis of the textured specimens. These were prepared by a powder metallurgical method [34] from 300 mesh powders.

2.4.3 Pole Figure Measurements

X-ray pole figures were measured using the reflection technique [6]. The equipment was a Siemens Texture Goniometer, a Kristalloflex IV X-ray generator, and a Kompensograph recorder. Copper K\(\alpha\) radiation, with a primary filter of nickel, was used for all measurements. The power setting was 16 mA. at 40 kV. A scintillation counter, coupled with a pulse height analyser, was used to measure the diffracted beam.

The texture goniometer has been described by Neff [52]. The specimen revolves about an axis normal to its surface and simultaneously about an axis in its surface coplanar with the incident and diffracted beams. In this way the diffracted X-ray intensity is measured along a spiral path in the stereographic projection, from which the pole figure is constructed. The goniometer was set up so that the pitch of the
spiral was $5^\circ$. This spiral for the composite specimens used is illustrated in Fig. 2.1.

The Bragg reflections measured were those from the \{200\}, \{220\}, and \{11\} planes. These are quite widely spaced in the materials tested, using Cu-K\alpha radiation, and the receiving slit for the scintillation counter could be opened wide without overlapping adjacent reflections. The defocussing effects at large specimen inclinations are thereby reduced [3,6]. Preliminary measurements with random powder samples indicated no detectable reduction in diffracted intensity at angles up to $65^\circ$ from the spiral centre. Since measurements up to $55^\circ$ are sufficient to cover a complete quadrant of the pole figure with the composite specimens used [8], it was unnecessary to use the random data to correct for defocussing.

The measured data were output in the form of a chart, the x axis corresponding to the angular coordinate, and the y axis to the diffracted intensity. It was required to convert these data into digital form for subsequent computer processing. A D-Mac pencil follower, type PF10000, was used for this purpose. This consists of a table with a servo - following mechanism beneath its surface, an electromagnetic 'pencil', a decoder unit, and a high speed paper tape punch. The chart was placed on the table, and the trace was followed with the pencil. The signal from the pencil was picked up by the following unit which relayed the position of the pencil to the decoder unit, and thence to the punch. Reference coordinates were also recorded in order to calculate the relation between the chart axes and the D-Mac axes.
Figure 2.1. The goniometer recording spiral for the composite specimens used for pole figure determination.

Figure 2.2. Illustrating the coordinates of a point P with respect to the sheet normal direction (ND), and with respect to the spiral centre (S).
2.4.4 Plotting of Pole Figures

In order to save labour, a computer program was written to plot pole figures from the tapes produced by the D-Mac pencil follower. Standard subroutines were available to draw contours on a rectangular or square array of data points. A 20 x 20 array of data points was set up to cover one quadrant of the pole figure, and the intensity at each point was allocated by linear interpolation from the four nearest data points on the recording spiral. In order to relate the coordinates of a point \( P \) relative to the pole figure with its coordinates relative to the offset plotting spiral, stereographic mapping equations are required. Elias and Heckler [8] have given equations, but they are unnecessarily cumbersome. The following equations were used:

\[
\tan \Theta = \frac{(2 \cot \frac{\pi}{2} \sin \phi)}{[\sin(\phi + \beta) - \cot \frac{\pi}{2} \sin(\phi - \beta)]} \\
= \frac{N}{D} \tag{2.1a}
\]

\[
\cos \psi = \cos \beta \cos \phi + \sin \beta \sin \phi \cos \alpha \tag{2.1b}
\]

where \( \Theta, \psi \), are polar coordinates relative to the pole figure, \( \phi, \alpha \), are the coordinates relative to the spiral, and \( \beta \) is the spiral offset (see Fig.2.2).

\( \psi \) lies in the range \( 0 - \pi \), and is uniquely determined by equation (2.1b). \( \Theta \) however, is in the range \( 0 - 2\pi \), but it is uniquely determined by the observation that \( N \) and \( D \) in equation (2.1a) have the sign of \( \sin \Theta \) and \( \cos \Theta \) respectively. This is a further advantage of equation (2.1) over those given by Elias and Heckler.

Provision was made in the program for the application of the defocussing correction by comparison with data from a random specimen, although this was not needed for the present study (see Section 2.4.3).
The data were normalised by integration over the whole pole figure, and contours were drawn at suitable intervals, using a Calcomp digital incremental curve plotter.

2.5 Mechanical Test Procedure

2.5.1 Elastic Modulus Measurements

The variation of Young's modulus in the plane of a rolled sheet is conveniently measured by the transverse resonant vibration method of Roberts and Nortcliffe [53]. Small rectangular specimens were suspended horizontally from two piezo-electric gramophone pick-ups. A signal generator was used to drive one pick-up, which excited vibrations in the specimen. These in turn excited the second pick-up, and the signal from this was fed into an oscilloscope. The resonant frequency of the specimen was indicated when the signal detected by the oscilloscope was a maximum. The Young's modulus is given by the formula [54]:

\[ E = 0.00095 \rho \left( \frac{l^2 f}{t} \right)^2 \text{ N/m}^2 \]

where \( l \) is the length of the specimen, mm
\( \rho \) is the specific gravity
\( t \) is the specimen thickness, mm
\( f \) is the fundamental resonant frequency, Hz

Specimens were cut from the rolled sheet at angular intervals of 15 degrees. The dimensions of the specimens were: length 40 mm, width 4 mm. These dimensions gave a fundamental resonance at about 700 Hz with specimens of typically 0.3 mm thickness. The specimens were suspended from the pick-ups by cotton loops. The applied frequency was varied to find the resonances, and the mode of vibration was determined by resting a light object on the specimen to locate the nodes. The fundamental resonance is characterised by two nodes, one near either end of the
specimen. The resonant frequency was measured with a crystal controlled frequency meter, and Young's modulus was calculated from the above formula.

2.5.2 Proof Stress Measurements

In order to measure the anisotropy of flow stress in the rolled sheet tensile test specimens were punched from the sheet at angular intervals of 15 degrees. The gauge length was 1 inch (25.4 mm) and the width 0.25 in. (6.3 mm). Tensile tests were performed with an Instron model TT testing machine. The crosshead speed was 5 mm/minute. It was not possible to use an extensometer on the specimens, so the crosshead displacement was taken as a measure of the strain in order to determine the 0.2 percent proof stress. The maximum machine deflection at the typical test load (100 Kg) was 0.01 mm, which would not significantly affect the results.

2.6 The Titan Computer

All of the more involved calculations performed in the course of this work were done on the Cambridge University Titan computer. This machine is a prototype of the I.C.T. Atlas II computer. The core store consists of 128k words (1k = 1024 words), the word length being 48 bits. This very large word size, coupled with a 72 bit accumulator, results in very small rounding errors during computation. There are a disc store with a 16 million word capacity, six magnetic tape decks, two line printers, and two curve plotters in addition to punched paper tape handling equipment. The administration of the computer is handled by a built in program, the Supervisor, in order to make the most efficient use of the facilities.
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The Supervisor also controls the operation of an on-line multiple access system, whereby users may have direct access to the computer via Teletype consoles. Up to twenty users may be on line at any one time. An on-line user may input information directly to the computer, and compile and run programs with a very short turn-round time. A variety of system programs are available, which are mainly concerned with the administration of the user's allocation of disc space, and with document handling and editing facilities. In addition, an on-line user may initiate jobs to be run later at the Supervisor's convenience (i.e. an off-line job). All jobs requiring input data from punched paper tape or magnetic tape must be run as off-line jobs, the computer operating staff being responsible for the input of paper tapes and the loading of magnetic tapes.

Most of the calculations performed in the course of this work took a sufficiently large amount of computation time, or produced such a large amount of output, that it was inconvenient to run the programs on-line. The on-line system was mainly used for editing and debugging programs, and for initiating jobs to be run off-line. All of the programs and important data were stored, in duplicate, on magnetic tapes.

Twelve compilers are available, which will accept most of the major scientific programming languages. All of the programs used in this work were written in Titan Autocode. This is a high level language with a structure based on the order code of the Atlas computer, and as a consequence of this the Autocode compiler is very fast and efficient.
3.1 Introduction

A collection of X-ray pole figures for a textured sample, although containing a great deal of information about the texture of the sample, does not reveal the crystallite orientation distribution directly since the correlations between the pole figures demanded by the crystal lattice structure are not brought out explicitly. Ideal orientations may be assigned which give a satisfactory agreement with the pole figure data, but except in cases where the texture is very sharp an unambiguous assignment is not usually possible. In these cases a quantitative representation of the crystallite orientation distribution may be obtained by a suitable analysis of pole figure data, taking due account of the crystal symmetry. The methods currently available are the analytical method due to Roe [44] and Bunge [45], and the iterative approach due to Williams [46]. The analytical methods have a certain advantage since data representing the texture of a sample may be stored conveniently as a set of coefficients (see Chapter 8). The methods of Roe [44] and Bunge [45], although differing in detail, are equivalent in principle. Roe's method is slightly more general in application, and he employs the notation usually found in English mathematical texts. Consequently Roe's method was used in this work for the analysis of pole figure data.

In the description of his method, Roe assumes a familiarity with the properties of the spherical harmonic functions. A detailed explanation of the method is given in this chapter, together with details of its practical application, and of certain extensions of it.
3.2 Roe's Method

The orientation of a crystallite in a polycrystalline sample is specified by means of the Euler angles $\psi, \Theta,$ and $\phi$ (Figs. 1.1 and 3.1). Using the convention of Roe, $\psi$ and $\Theta$ are the polar coordinates of the crystal $z$ axis with respect to the sample axes, and $\phi$ describes the rotation of the crystal about its $z$ axis. Substituting these angles in equation (1.1) the orientation distribution function for the crystallites is represented by $w(\psi, \xi, \phi)$, where $\xi = \cos \Theta$ and

$$
\int_0^{2\pi} \int_0^\pi \int_0^\pi w(\psi, \xi, \phi) \, d\xi \, d\psi \, d\phi = 1
$$

The experimentally observed data consist of a set of functions $q_i(\xi, \eta)$ describing the orientation distribution of the normals to the $i$th crystal plane with respect to the sample axes (where $\cos^{-1} \xi$ is the polar, and $\eta$ the azimuthal angle). These data are expanded in a series of spherical harmonics:

$$
q_i(\xi, \eta) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Q_{lm} P_l^m(\xi) e^{-im\eta} \quad (3.1)
$$

where $Q_{lm}$ are coefficients, and $P_l^m$ are normalized associated Legendre polynomials. Since the associated Legendre polynomials form an orthogonal set with respect to $1$

$$
i.e. \quad \int_{-1}^{1} P_l^m(\xi) P_{l'}^{m'}(\xi) \, d\xi = 1, \, l = l' \quad \int_{-1}^{1} P_l^m(\xi) P_{l'}^{m'}(\xi) \, d\xi = 0, \, l \neq l'
$$

the coefficients are obtained in an analogous way to the determination of the coefficients in a Fourier series:
Figure 3.1. The Euler angles $\psi, \theta, \phi$, relating the specimen axes RD, TD, ND, with the crystal axes x, y, z.
\[ Q_{lm} = \frac{1}{2\pi} \int_{-1}^{1} q(\xi, \eta) P_l^m(\xi) e^{im\phi} \, d\xi \, d\eta \quad (3.2) \]

The crystallite orientation distribution function is expanded similarly into a series of generalized spherical harmonics,

\[ w(\psi, \xi, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} W_{lmn} Z_{lmn}(\xi)e^{-im\psi -in\phi} \quad (3.3) \]

where \( Z_{lmn} \) is a generalization of the associated Legendre function, and \( W_{lmn} \) are coefficients. The problem is one of finding the relation between the sets of coefficients in the respective series.

To do this it is convenient to define a new set of axes \( x_i, y_i, z_i \), in the crystal, so that the \( z_i \) axis coincides with the particular plane normal considered. The distribution function with respect to these axes is \( w'(\psi', \xi', \phi') \). Since from the definition of the Euler angles (see Fig. 3.1) \( \psi' \) and \( \xi' \) are the polar coordinates of the \( z_i \) axis with respect to the sample, \( \psi' = \eta \) and \( \xi' = \zeta \). From Equation (1.3)

\[ q_i(\xi, \eta) = \int_{0}^{2\pi} w'(\xi, \eta, \phi') \, d\phi' \quad (3.4) \]

The axes \( x_i, y_i, z_i \), are related to the original axes \( x, y, z \), by the Euler angles \( \Phi_i, \Theta_i, \) and \( \Lambda_i \), where \( \Phi_i \) and \( \Theta_i \) are the polar coordinates of the \( i \)th plane normal with respect to the original crystal axes, and \( \Lambda_i \) has any convenient value. If the coefficients of the expansion of \( w'(\xi, \eta, \phi') \) are \( W_{lmn} \), then the relation between the \( W_{lmn} \) and the \( W'_{lmn} \) is given by the Legendre addition theorem,

\[ W'_{lmn} = \left( \frac{2}{2l+1} \right)^{\frac{1}{2}} \sum_{p=-l}^{l} W_{lmp} Z_{lmn}(\cos \Theta_i) e^{ip\Phi_i} e^{in\Lambda_i} \quad (3.5) \]
Substituting the series expansions for \( q_i(\xi, \eta) \) and \( w'(\xi, \eta, \phi') \) in equation (3.4) we obtain:

\[
\sum_{l=0}^{\infty} \sum_{m=-l}^{l} Q_{lm}^i P_l^m(\xi) e^{-im\eta} = \int_{0}^{2\pi} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} W_{lmn}^i Z_{lmn}(\xi) e^{-im\eta} e^{i\phi'} d\phi' = 2\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} W_{lm0}^i Z_{lm0}(\xi) e^{-im\eta}
\]

and by comparison,

\[
Q_{lm}^i = 2\pi W_{lm0}^i
\]

Substituting from equation (3.5), and noting that \( Z_{lm0}(\xi) = P_l^m(\xi) \), we obtain

\[
Q_{lm}^i = 2\pi \left( \frac{2}{2l+1} \right) \sum_{p=-l}^{l} W_{lmp}^i P_l^p(\cos \Theta) e^{ip\phi_i}
\]

Equation (3.6) (Roe's[44] equation (13)) represents, for a given value of \( l \), a set of linear simultaneous equations, with \( 2l + 1 \) unknowns. However, the effect of crystal and specimen symmetry is to restrict the possible values of \( Q_{lm} \) and \( W_{lmn} \). In particular, for cubic crystal symmetry and orthotropic specimen symmetry, \( Q_{lm} \) and \( W_{lmn} \) are all real,

\[
W_{lmn} = Q_{lm} = 0 \text{ when } l = 2
\]

or

\[
l \neq 2k
\]

or

\[
m \neq 2k
\]

or

\[
n \neq 4k
\]

where \( k \) is an integer

\[
W_{lmn} = W_{lm\bar{n}} = W_{l\bar{m}n} = W_{l\bar{m}\bar{n}}
\]

\[
Q_{lm} = Q_{l\bar{m}}
\]

and, for given values of \( l \) and \( m \), the \( W_{lmn} \) are linearly related [48].

The effect of these restrictions for the particular case considered is
that all the coefficients up to and including 22nd order \((1 = 22)\) may be
determined from two pole figures. Because the \(Q_{lm}\) and \(W_{lmn}\) are all real,
equations (3.1), (3.2), (3.3), and (3.6) become:

\[
q_i(\xi, \eta) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Q_{lm} P_l^m(\xi) \cos m\eta \tag{3.7}
\]

\[
Q_{lm} = \frac{1}{2\pi} \int_{0}^{2\pi} \int_{-1}^{1} q_i(\xi, \eta) P_l^m(\xi) \cos m\eta \, d\xi \, d\eta \tag{3.8}
\]

\[
w(\psi, \xi, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} W_{lmn} Z_{lmn}(\xi) \cos(m\psi + n\phi) \tag{3.9}
\]

\[
Q_{lm} = 2\pi \left( \frac{2}{2l+1} \right)^{1/2} \sum_{p=-l}^{l} W_{lm0} P_l^p(\cos \Theta) \cos p\phi \tag{3.10}
\]

Equation (3.10) serves not only to define the simultaneous
equations relating the observed data with the distribution function, but
can also be used to generate the pole figures corresponding to any
desired crystal plane by substituting the appropriate coordinates.
Regeneration of the pole figures from which the original data were
obtained can be used as a check on the fidelity of the distribution
function.

3.3 Practical Application of Roe's Method

In the application of equation (3.8) to experimental data, it is
convenient to replace the integration by summation over a finite number
of data points [49]. If the measured value \(q_i(\xi, \eta)\) is assumed to
represent the interval \((\xi_K, \eta_K)\), then equation (3.8) becomes
\[ q_{lm} = \frac{1}{2\pi} \sum_{K} q_{l}(z_K^+, z_K^-) \int_{z_K^+}^{z_K^-} \int_{\eta_K^+}^{\eta_K^-} P_1^m(\xi) \cos(m\eta) \, d\eta \, d\xi \]

where \( z_K^+, z_K^- \) designate the upper and lower limits of the \( k \)th interval. In this work the \( q_{l}(z, \eta) \) were determined at each of 324 data points, corresponding to a 5 degree interval in \( z \) and \( \eta \), by linear interpolation from the four nearest data points on the goniometer plotting spiral.*

* Many workers, using the Schultz reflection method for pole figure determination [6] determine only the central 70 - 80 degrees of the pole figure. Such (incomplete) pole figures cannot be used to determine the orientation distribution function, since no information is given about the fourth order coefficients \( W_{4mn} \).

The assumption of orthotropic specimen symmetry is convenient since it reduces the amount of computation involved in the analysis by a factor of (roughly) sixteen. For this reason the composite specimens were constructed to give an average pole figure for the four quadrants (see Chapter 2, section 2.4.1).

By measuring more pole figures than necessary for a given value of \( l \), equation (3.10) may be overdetermined and solved by a least squares method [44]. An estimate of the error in the coefficients \( Q_{lm} \) and \( W_{lmn} \) may then be made. From the results of other workers [11,23], and from preliminary tests, it is apparent that the coefficients become zero within experimental error at typically between 16th and 22nd order. Since the amount of computation involved in the analysis increases
roughly as the square of the number of orders considered, it is necessary to truncate the series at a value of 1 which gives adequate accuracy without an excessive computation time. In this work the series were evaluated up to and including 20th order.

There are a variety of generating formulae which may be used to evaluate the spherical harmonic functions $P_n^m(\tilde{\xi})$ and $Z_n^m(\tilde{\xi})$ [47]. Morris and Heckler [49] have used a multiple angle form which is relatively immune from rounding errors in computation, but which involves the storage of a large amount of tabulated data. Since the word size of the Atlas II computer used in the present work is greater than that of most computers (i.e. 13 decimal digits as opposed to typically 7 or 8 decimal digits) it was possible to use a recursive power series expansion without undue rounding error (the error was $\ll 0.1$ percent at 20th order). The generating formulae used were those given by Roe [44], equation (A3).

For a specimen with cubic crystal symmetry and orthotropic specimen symmetry, all essentially distinct orientations are contained in the range:

$$0 \leq \psi \leq \pi/2$$
$$0 \leq \phi \leq \pi/2$$
$$0 \leq \theta \leq \tan^{-1}(1/\cos \phi), \quad \phi \leq \pi/4$$
$$0 \leq \theta \leq \tan^{-1}(1/\sin \phi), \quad \phi > \pi/4$$

It is more usual, however, to compute the function in the range

$$0 \leq \psi \leq \pi/2$$
$$0 \leq \phi \leq \pi/2$$
$$0 \leq \theta \leq \pi/2$$

as in this way the inter-relations between the orientation maxima are more clearly seen. The function is usually plotted as iso-intensity
contours against $\Theta$ and $\Psi$, for various constant values of $\phi$, although other sections may, of course, be used. In order to be consistent with pole figure and inverse pole figure practice, the function is normalized so that a value of unity corresponds to uniform orientation distribution.

3.4 Estimation of Errors

3.4.1 Experimental Errors

The measured pole figures will be liable to experimental errors for a variety of reasons. For example, errors are introduced by inaccuracies in specimen preparation and mounting, by statistical variations in the X-ray beam, fluorescence of the specimen caused by high energy radiation which penetrates the filter, and by Bragg reflection of the background radiation. Further errors can be introduced at the data processing stage, for example when digitizing the X-ray data using the D-Mac pencil follower. While every effort is made to minimise these errors, it is necessary to know to what extent they occur.

Bunge and Haessner [11] suggest that, for cubic crystals, the effect of experimental errors may be judged from the magnitude of the second order coefficients of the pole figure expansion, since all second order coefficients should be identically zero for these materials. Using this criterion they have shown that the experimental errors in pole figures measured by combined transmission and reflection methods are very large (up to 39 percent). Bunge and Haessner suggest that a better indication of the accuracy of pole figure measurements may be obtained by comparison of the compatibility of the various pole figures with each other when equation (3.10) is over determined, by comparing the probable
errors in the coefficients with the mean absolute values of the coefficients of the same order.

In all of the work described in this dissertation, three pole figures were measured. This means that equation (3.10) was over determined for all values of \( l \) considered. The probable errors in the coefficients in the respective series were calculated, and the effects of these errors on the pole figures and orientation distribution function were calculated by the following method.

If the probable error in \( Q_{lm} \) is \( \Delta Q_{lm} \), then the probable difference between the actual and measured pole figure is:

\[
\Delta Q_e = \sum_{l=0}^{\infty} \sum_{m=L}^{l} Q_{lm} P_{l}^m(\zeta) e^{-im\eta} - (Q_{lm} - \Delta Q_{lm}) P_{l}^m(\zeta) e^{-im\eta}
\]

\[
= \sum_{l=0}^{\infty} \sum_{m=L}^{l} \Delta Q_{lm} P_{l}^m(\zeta) e^{-im\eta}
\]

The mean error over all orientations is given by:

\[
q = (1/4\pi \int \int \sum_{l=0}^{\infty} \sum_{m=L}^{l} \Delta Q_{lm} \Delta Q_{lm}^* [P_{l}^m(\zeta)]^2 \, d\zeta \, d\eta
\]

\[
= \left(1/2\right) \sum_{l=0}^{\infty} \sum_{m=L}^{l} \Delta Q_{lm} \Delta Q_{lm}^*
\]

where \( * \) denotes the complex conjugate.

The similar result for the error in the orientation distribution function is:

\[
v = \left(1/2\right) \sum_{l=0}^{\infty} \sum_{m=L}^{l} \sum_{n=L}^{l} \Delta W_{lmn} \Delta W_{lmn}^*
\]

The errors given by these expressions are, in fact, low estimates since the coefficients are determined by integration over the pole figures, and it is possible that errors in the pole figures.
partially compensate. It is also possible that errors may be present which cause no incompatibility between the pole figures. These would not show either in the above method, or in the presentation used by Bunge.

3.4.2 Truncation Errors

The expansions of the pole figure data, and of the orientation distribution function are infinite series. In practice it is necessary to truncate the series after a finite number of terms. The error in the pole figure expansion due to truncation at \( l = \lambda \) may be determined easily as the measured function is available for comparison with the series expansion. The truncation error is given by:

\[
\sigma = \left( \frac{1}{4\pi} \right) \left[ \int_0^{2\pi} \int_0^{\pi} \left( q(\zeta, \eta) - \sum_{l=0}^{\lambda} \sum_{m=-l}^{l} Q_{lm} P_l^{m}(\zeta) e^{-im\eta} \right)^2 d\zeta d\eta \right]
\]

\[
= \left( \frac{1}{4\pi} \right) \left[ \int_0^{2\pi} \int_0^{\pi} \left[ \int_0^{2\pi} \int_0^{\pi} \left[ q(\zeta, \eta) \right] d\zeta d\eta - 2\pi \sum_{l=0}^{\lambda} \sum_{m=-l}^{l} Q_{lm} P_l^{m} \right] \right]
\]

The truncation error in \( w(\psi, \xi, \phi) \) is more difficult to estimate as the series expansion is the only estimate available of the actual function. The truncation error is given by:

\[
\sigma_{\omega T} = \left( \frac{1}{8\pi^2} \right) \left[ \int_0^{2\pi} \int_0^{\pi} \int_0^{2\pi} \left[ \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} W_{l,m,n} Z_{l,m,n}(\zeta) e^{-im\psi} e^{-in\phi} \right] d\zeta d\psi d\phi \right]
\]

\[
= \frac{1}{2} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} W_{l,m,n} W_{l,m,n}^{*}
\]

The product \( W_{l,m,n} W_{l,m,n}^{*} \) may be estimated by extrapolation from the known values. The estimate of the truncation error obtained in this way can be misleading since a large value may appear to indicate that a better fit
would be obtained by considering more terms in the series. In fact no useful purpose is served by extending the series once the experimental error is of the same magnitude as the coefficients. Furthermore, even if the experimental errors were trivial, the order at which the series is truncated must be related to the 'resolving power' of the method used to determine the pole figure (e.g. if the pitch of the scanning spiral on the texture goniometer is 5 degrees, there is no point in extending the series beyond about 36 orders).

3.5 Interpretation of the Distribution Function

The results of analyses of crystal orientation distributions are normally represented graphically by plotting the probabilities in Euler space and taking constant sections of one of the Euler angles, most usually constant $\phi$ sections. The texture components can be considered in terms of ideal orientations $(hkl)[uvw]$. In cubic crystals these correspond to the Euler angles given by

$$\cos \psi = \frac{w}{(u^2 + v^2 + w^2)^{\frac{1}{2}}} \frac{(h^2 + k^2 + l^2)^{\frac{1}{2}}}{(h^2 + k^2)^{\frac{1}{2}}} \quad (h,k \neq 0)$$

$$\cos \theta = \frac{1}{(h^2 + k^2 + l^2)^{\frac{1}{2}}}$$

$$\cos \phi = \frac{h}{(h^2 + k^2)^{\frac{1}{2}}} \quad (h,k \neq 0)$$

For the case in which $h = k = 0$

$$\cos(\psi + \phi) = \frac{u}{(u^2 + v^2 + w^2)^{\frac{1}{2}}}$$

Alternatively, an ideal orientation can be found from known Euler angles using
\[ h = -\sin \theta \cos \phi, \quad k = \sin \theta \sin \phi, \quad l = \cos \theta \]
\[ u = \cos \psi \cos \Theta \cos \phi - \sin \psi \sin \phi \]
\[ v = -\cos \psi \cos \Theta \sin \phi - \sin \psi \cos \phi \]
\[ w = \cos \psi \sin \Theta \]

and rationalizing the resulting indices. Davies et al. [55] have given charts indicating the Euler angles corresponding to low index ideal orientations in the cubic system.

The volume fraction of crystallites having an orientation within a given region of Euler space may be determined by integration of the distribution function over that region. In particular it would be convenient to determine the volume fraction of crystallites associated with a given ideal orientation \((hkl)[uvw]\). If the particular ideal orientation considered is described by the Euler angles \(\Theta, \Psi, \Phi\), and we wish to determine the volume fraction of crystals whose normal direction is within \(\gamma_N\) of the ideal normal direction, the limits of integration on \(\Theta\) and \(\Phi\) are given by

\[ \Theta_i - \gamma_N \leq \Theta \leq \Theta_i + \gamma_N \]
\[ \Phi_i - \delta \leq \Phi \leq \Phi_i + \delta \]

where \(\delta = \cos^{-1}\left(\frac{\cos \Theta_i - \cos \Theta_i \cos \Phi_i}{\sin \Theta \sin \Theta_i}\right)\)

For a given \(\Theta\) and \(\Phi\), \([uvw]\) will, in general, be rotated away from the rolling plane, but will be within \(\gamma_N\) of it. The \(\psi'\) necessary to bring \([uvw]\) nearest the rolling direction is given by

\[ \psi' = \psi_i - \tan^{-1}(\tan \alpha \cos \xi) \]
where \(\cos \alpha = \cos^2 \beta + \sin^2 \beta \cos(\Phi - \Phi_i)\)
\(\cos \beta = \cos \psi_i \sin \Theta\)
\(\xi = \frac{\pi}{2} - \cot^{-1}(\sin \psi_i \tan \Theta) - \sin^{-1}\left[\frac{\sin(\psi - \Phi) \sin \beta}{\sin \alpha}\right] \)
\[
\begin{align*}
    h &= -\sin \Theta \cos \phi, \\
    k &= \sin \Theta \sin \phi, \\
    l &= \cos \Theta \\
    u &= \cos \psi \cos \Theta \cos \phi - \sin \psi \sin \phi \\
    v &= -\cos \psi \cos \Theta \sin \phi - \sin \psi \cos \phi \\
    w &= \cos \psi \sin \Theta
\end{align*}
\]

and rationalizing the resulting indices. Davies et al. [55] have given charts indicating the Euler angles corresponding to low index ideal orientations in the cubic system.

The volume fraction of crystallites having an orientation within a given region of Euler space may be determined by integration of the distribution function over that region. In particular it would be convenient to determine the volume fraction of crystallites associated with a given ideal orientation \((hkl)[uvw]\). If the particular ideal orientation considered is described by the Euler angles \(\Theta, \psi, \phi\), and we wish to determine the volume fraction of crystals whose normal direction is within \(\gamma_n\) of the ideal normal direction, the limits of integration on \(\Theta\) and \(\phi\) are given by

\[
\begin{align*}
    \Theta_i - \gamma_n &\leq \Theta \leq \Theta_i + \gamma_n, \\
    \phi_i - \delta &\leq \phi \leq \phi_i + \delta
\end{align*}
\]

where \(\delta = \cos^{-1}\left(\frac{\cos \gamma_n - \cos \Theta \cos \Theta_i}{\sin \Theta \sin \Theta_i}\right)\)

For a given \(\Theta\) and \(\phi\), \([uvw]\) will, in general, be rotated away from the rolling plane, but will be within \(\gamma_n\) of it. The \(\psi'\) necessary to bring \([uvw]\) nearest the rolling direction is given by

\[
\psi' = \psi_i - \tan^{-1}\left(\tan \alpha \cos \xi\right)
\]

where \(\cos \alpha = \cos^2 \beta + \sin^2 \beta \cos(\phi - \phi_i)\)

\[
\begin{align*}
    \cos \beta &= \cos \psi_i \sin \Theta \\
    \xi &= \frac{\pi}{2} - \cot^{-1}\left(\sin \psi_i \tan \Theta\right) - \sin^{-1}\left(\frac{\sin(\phi - \phi_i) \sin \beta}{\sin \alpha}\right)
\end{align*}
\]

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If the number of crystals with their rolling direction within $\Psi_k$ of [uvw] is required, the limits of integration for $\Psi$ will be

$$\Psi' - \Psi_k \leq \Psi \leq \Psi' + \Psi_k$$

ignoring the rotation of [uvw] out of the rolling plane. This technique has been used by Kallenl and Davies[56] who studied the distribution of crystallites around the $\{110\}<112>$ ideal orientation in $\alpha$-brass.

3.6 Severity of Texture

The extent to which the crystallites have taken up a given ideal orientation can be investigated by the method described in section 3.5. It would be informative, however, to have a measure of the severity of the texture in a given sample which is independent of the type of texture. Sturcken and Croach [57] suggested such a parameter, determined from inverse pole figure measurements, and applied it to rolled uranium rods. Their parameter is only suitable for fibre textures, and is not independent of the type of texture in samples exhibiting lower symmetry.

A suitable parameter is the standard deviation of the orientation distribution function from uniformity. This is given by

$$(SP) = \left(\frac{1}{8\pi^2}\right) \int \left[ w(\omega) - \left(\frac{1}{8\pi^2}\right) \right]^2 d\omega$$

where $\omega$ is a general orientation.

Because of the orthogonality of spherical harmonics:

$$ (SP) = \left(\frac{1}{8\pi^2}\right) \left[ \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} W_{lmn}^* W_{lmn} - \left(\frac{1}{8\pi^2}\right) \right] $$

and since $W_{000} = 1/4\pi^{3/2}$

$$ (SP) = \left(\frac{1}{8\pi^2}\right) \left[ \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} W_{lmn}^* W_{lmn} \right] $$
If the parameter is normalized so that uniformity corresponds to unity,

\[ (SP) = 4\sqrt{2} \pi^2 \left( \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} W_{l,m,n} W_{l,m,n}^* \right)^{1/2} \]

This parameter may be computed readily from the \( W_{l,m,n} \). Truncation error is small since the product \( W_{l,m,n} W_{l,m,n}^* \) converges rapidly in practice. Providing that \( SP \) is always computed to the same order it can form a basis for the quantitative comparison of the rate of texture formation in different materials.
PART II

DEVELOPMENT OF ROLLING TEXTURE

IN COPPER AND α-BRASS
4.1 Introduction

It has long been recognised that the rolling texture of silver or α-brass is not exactly the same as that of copper or many other fcc metals. The quantitative pole figure determinations of Beck and co-workers [58, 59] suggested that the texture of brass could be characterized by the ideal orientations \{110\}<112> with a \{110\}<001> minor component, while the copper texture was best described as \{123\}<412> plus \{146\}<211>. Subsequent work on copper has resulted in a variety of descriptions of the rolling texture [2, 4], illustrating that a range of orientations is present from \{110\}<112> to \{112\}<111>.

Since the rolling texture of a metal reflects the operative deformation mechanisms, the difference in rolling texture between, for example, copper and aluminium on the one hand, and silver and α-brass on the other, has attracted a great deal of research and speculation. Barrett and Massalski [2] and Dillamore and Roberts [4] have recently reviewed many of the experimental findings. Certain specific subjects are reviewed in this chapter which are considered significant in the understanding of texture formation in fcc metals.

4.2 The Texture Transition in fcc Metals

4.2.1 Texture Transition by Alloying

The fact that α-brass exhibits a rolling texture which is different from that of pure copper suggests that alloying has been the
cause of this behaviour. The effect of solute additions was investigated by Smallman [60] and by Liu and Richman [61,62]. They showed that, for a given solute, a minimum amount is needed to initiate the transition, and the degree of transition increases with increasing solute content until complete transition is achieved. After this further solute additions have little effect. Liu and Alers [63] followed the texture transition in the copper - α-brass system by Young's modulus methods. They found that the transition took place in the range 4 - 10 weight percent in these alloys.

4.2.2 Texture Transition by Changing the Deformation Temperature

The effects of deformation temperature and heat treatment prior to cold rolling were investigated by Smallman [60] who showed that Cu - 5 percent Zn gave the copper type texture at 200°C, whereas rolling at -183°C gave rise to the brass type texture. Mueller [64] showed that pure copper deformed at -183°C gave rise to the brass type texture, while Hu et al. [65,66] demonstrated that silver rolled at high temperature gave rise to the copper type texture.

4.2.3 Texture Transition by Changing the Deformation Rate

Leffers [67] has investigated the textures of a Cu - 5 percent Zn alloy after rolling at various speeds. His results indicate that the texture changes towards the brass type at high deformation rates. Leffers has also obtained a value for the activation energy for the texture transition of 10 kcal/mole.
4.2.4 Texture Transition Related to Stacking Fault Energy

Hu and co-workers [65, 66, 68] have shown in a variety of systems that the brass type texture is associated with a high stacking fault frequency while the copper type texture was associated with a low stacking fault frequency. Smallman and Green [69] showed that the texture transition in copper alloys was related to the stacking fault energy, the copper type texture being associated with a high stacking fault energy metals, and the brass type texture with metals with a low stacking fault energy. This correlation between texture and stacking fault energy has been used by Dillamore et al. to determine stacking fault energies [70].

4.3 Development of Rolling Textures in fcc Metals

4.3.1 Single Crystals

Haessner [71] and Hu, Cline and Goodman [72] have recently reviewed the evidence relating to the stability of single crystals during rolling. Many of the earlier studies simply established the stable end orientation for a crystal with a particular initial orientation without recording the exact path of the crystal reorientation or the mechanisms giving rise to it. For example, Verbraak [73] found that a (112)[111] crystal of silver reoriented to (111)[112] and then to (110)[001]. He concluded that this was due to slip on (111)[011]. Hu et al. [72] have since shown that this reorientation is due to twinning, with subsequent slip.

Hu et al. rolled crystals of copper, and Cu - 4 percent Al, having initial orientations of (110)[112] and (112)[111]. The (110)[112] crystal of copper was stable to 99 percent reduction, whereas the alloy crystal with this orientation assumed a double {110}<112>
texture at this reduction although it had been stable until 95 percent reduction. The behaviour of the (112)[111] crystals of different composition was markedly different even at small reductions. While the copper crystal retained its initial orientation at 50 percent reduction, the alloy crystal developed a large orientation spread and a strong component of the (552)[115] twin orientation. At 95 percent reduction a minor twin component had formed in the copper crystal, while the alloy crystal had undergone reorientation of both its matrix and twin portions to (111)[112] and (110)[001] respectively. These results are comparable with those of Ahlborn et al. [74] for a (112)[111] silver crystal.

Heye and Wasserman [75] performed tests on crystals of silver with several initial orientations, and concluded that twinning would occur in crystals whose orientation satisfied certain empirical criteria, and that twinning was most likely in the (112)[111] orientation. Chin et al. [76] showed that the experimental results of Heye and Wassermann could be explained by an extension of the Taylor analysis [77] of polycrystalline deformation to the case of mixed slip and twinning. Wonsiewicz and Chin [78] have shown that deformation banding (the splitting of a crystal into several components which then deform independently) could also be explained by the Taylor analysis provided that each region of the crystal was treated separately.

The overall picture which emerges from single crystal deformation is that for crystals of a metal which forms the copper type texture the initial orientations which correspond to elements of the polycrystalline deformation texture are all stable to high deformations. For metals which form the alloy texture, crystals of all orientations except (110)[112] have been found to be unstable, breaking down either by twinning or by the formation of deformation bands. Even the
\{110\}<112> crystal of Cu - Al rolled by Hu et al. [72] showed signs of instability at 99 percent reduction.

4.3.2 Polycrystalline Aggregates

The development of rolling textures in aluminium and silver was studied by Dillamore and Roberts [79] who found that the initial texture build-up was towards the alloy type in both materials, with silver continuing towards this texture until at least 99 percent deformation. The aluminium was found to change from the alloy type texture to the pure metal type texture at fairly high deformations. On the other hand, later work by Hu et al. [72] indicated that in both copper and brass the initial texture build-up was towards the copper type texture, with subsequent deviation by the brass towards the alloy type texture. Dillamore, Butler and Green [80] confirmed this latter tendency in copper - aluminium alloys, and concluded that the starting material of Dillamore and Roberts must have deviated sufficiently from random to influence the texture development.

Kamijo and Sekine [81] chose highly textured sheets of copper as their starting material, and rolled them at various temperatures. A sheet with \{112\}<111> initial texture, and rolled at -196°C, showed a decrease in this component, and a corresponding increase in the twin orientation. Conversely, a sheet which had been rolled at -196°C to give the alloy texture was then rolled 92 percent at 100°C, when very little build-up of the \{112\}<111> 'pure metal' texture component was observed.

A combined microstructural and X-ray investigation of the texture development in copper and Cu - 15 percent Zn was undertaken by Leffers and Grum Jensen [82]. They observed that the initial texture development was similar in both materials, towards the pure metal type...
texture. At higher reductions (about 65 percent) the brass developed the alloy texture. Their microstructural observations showed that copper rolled at room temperature produced a pronounced sub-grain structure. In brass rolled 50 percent a few twins were observed, and extensive twinning was found at 65 percent reduction. Similar results were obtained with copper rolled at -196°C. The orientations of the twins were not found to correspond to any major component of the observed pole figures.

4.4 Theories of Texture Development in fcc Metals

4.4.1 Early Theories

The fact that the deformation textures of fcc metals and alloys are different has lead to a great deal of speculation about the reasons for the texture transition. Early theories (see [1]) have largely been abandoned or absorbed into more recent theories as experimental evidence relating to the texture transition has accumulated.

4.4.2 Texture transition due to Deformation Twinning

Wassermann [83] proposed that the rolling texture of fcc metals can be considered as being two limited fibre textures. One of these is based on the \{110\}<112> orientation, and the other on the \{112\}<111> orientation. If mechanical twinning is a possible deformation mode in materials with a low stacking fault energy then the texture components near \{112\}<111> can be converted by twinning to orientations near \{552\}<115>, which rotate into the \{110\}<001> orientation by subsequent slip. The \{110\}<112> based fibre texture retains its orientation during deformation because twinning would lead to shape changes that do not conform with the rolling process. The predictions of the twinning theory
have been largely supported by experiments on single crystals [72,74,75] although Leffers [84] has questioned the validity of single crystal results when applied to polycrystalline aggregates. Recent pole figure evidence [72,80] relating to the development of textures in materials exhibiting both the pure metal and the alloy type textures has indicated that the characteristics of the pure metal texture develop first, and that the alloy characteristics are developed at higher deformations, in accordance with the twinning theory.

Direct evidence of twinning in low stacking fault energy fcc alloys has been produced by Hu et al. [72], Leffers and Grum Jensen [82] and by Turley [85]. Leffers [82,84,86] indicates that the orientations of the twins that were observed were not in accordance with Wassermann's theory, and he considers that they serve only to scatter the texture. Heye and Wassermann, in their reply, maintained that Leffers' results were in accordance with their theory [87].

Williams [46] determined biaxial pole figures for 92 percent cold rolled aluminium, copper, and α-brass. He concluded that twinning was not important in the production of deformation textures in these materials. His interpretation of his results was incorrect, however, since he confused the initial and final orientations of the twinning process, as may be seen from the results of Chin et al. [76]. His results are, in fact, consistent with the twinning theory, showing a decrease in the \( \{112\}<111> \) component and an increase in the \( \{552\}<115> \) component in going from aluminium to copper to brass.
4.4.3 Texture Transition due to Cross Slip

Smallman and Green [69] and Dillamore and Roberts [72] suggested that the cause of the texture transition was the change in the cross slip behaviour of dislocations with stacking fault energy and temperature. The ease of cross slip depends on the stacking fault energy of the metal and on the temperature at which the deformation is taking place [68]. Dillamore and Roberts claimed that the alloy type texture \{110\}<112> was developed first, by normal (single) slip processes. For metals with high stacking fault energy, cross slip will then cause reorientation to give the pure metal texture. Since the stacking fault energy of a metal is lowered by alloy additions, and since cross slip can be activated by thermal energy, the cross slip theory appears to be consistent with both the temperature and composition dependence of the texture transition in fcc metals and alloys.

The cross slip theory in its original form is inconsistent with many observations. Abundant cross slip has been observed in brass at low deformations [89] and multiple slip is observed in copper even in the microstrain region [90]. The sequence of texture development observed in copper and copper alloys by Hu et al. [72] and by Dillamore et al. [80] is contrary to the simple cross slip theory, and reorientation of \{110\}<112> textured sheets of copper rolled by Kamijo and Sekine [81] was only very slow.

Leffers [91] has proposed a modified cross slip theory. According to Leffers, when primary dislocations approach a grain boundary the resultant stress concentration causes multiple slip in the grain boundary region, while the grain interior deforms by single slip to give the brass type texture. If cross slip is possible the stress concentrations are relieved and multiple slip has to occur throughout
the grain to maintain continuity. This multiple slip process leads to
the copper type texture. Leffers has produced simulated pole figures
based on these mechanisms (although his empirical approach to the
multiple slip problem has no theoretical justification). The predicted
copper textures are in reasonable agreement with experiment, but the
predicted brass textures fail to account for many of the observed
features (such as the region of fairly high intensity in the centre of
the (111) pole figure).

A weakness of this theory is that it predicts rapid rotations to
the stable end orientations for materials that do not cross slip. This
is not observed in practice, since one of the most prominent features of
the alloy texture is that it is not as sharp as the pure metal texture
at the same reduction [58,59]. Furthermore, multiple slip is observed in
brass even at low deformations [85]. In support of his theory Leffers
states that the observed activation energy for the texture transition
[67] is in agreement with that expected for the cross slip process [92].
However, the expected activation energy for dislocation intersection
[93] is also of the same order of magnitude, and depends in the same way
on stacking fault energy, so Leffers results are not unequivocal.

Related to the cross slip theory of the texture transition is a
theory due to Haessner [94]. He considered that the \{110\}<112> texture
was the end point for 'normal' slip rotations, and considered that slip
on \{001\} planes, so called 'cubic slip', was responsible for the
formation of the pure metal texture. Cubic slip is geometrically
equivalent to equal proportions of primary slip and cross slip [4] so
the macroscopic predictions of the cross slip theory and the cubic slip
theory are similar.
Hu, Cline, and Goodman [66] observed that the texture transition in silver was accompanied by a change in the stacking fault frequency, and further observations confirmed this correlation in other systems [68,72]. This led these workers to conclude that the texture transition was caused by the change in the deformation faulting behaviour per se. For energetic reasons a \( \{11\}<110> \) dislocation in a fcc crystal is usually split into two Shockley partial dislocations of the \( \{11\}<112> \) type. These are connected by a strip of stacking fault whose width is inversely proportional to the stacking fault energy of the material. (The width of the stacking fault is in fact proportional to the value of \( Gb/\gamma \), where \( \gamma \) is the stacking fault energy, \( G \) the shear modulus, and \( b \) the Burgers vector of the dislocation. In a given system variations of \( G \) and \( b \) are of secondary importance). The separated partial dislocations usually glide in a correlated sequential movement leading to the same result as normal \( \{11\}<110> \) slip. If the partials become widely separated the texture development may be altered because the effective slip direction is switched from \( <110> \) to \( <112> \).

Hu et al. [72] appear to consider independent motions of both partials equally likely. In effect, however, only the leading partial is likely to do so [95] since overtaking by the trailing partial would lead to extrinsic faulting [93] which is energetically unfavourable. This means that at most only one partial per plane can move in this way, as otherwise the sequential motion of the trailing partial results in effective \( <110> \) slip. If the motion of partial dislocations is such that a stacking fault is generated on successive \( \{11\} \) planes, the result is a deformation twin. In order that the stacking fault theory should not degenerate into the twinning theory the one partial per plane maximum
must be revised downwards. It is not thought likely that the limited amount of deformation available by this mechanism can account completely for the texture transition [80].

Besides the direct effect of stacking fault formation on deformation textures as envisaged by Hu et al., the interaction of stacking faults with other deformation modes has been considered by Chin [95], by Dillamore and Stoloff [96] and by Dillamore [97]. Stacking fault formation, by creating an effective forest, will tend to minimise dislocation activity on intersecting systems, and raise the stress required to continue deformation. Stacking faults will also act as effective nuclei for twins [93].

4.4.5 Texture Transition due to Dislocation Interaction

A theory of the fcc texture transition based on dislocation interactions has been proposed by Liu [98]. He considers that two flow mechanisms are operative during deformation. One mechanism, A, leads to the end orientation \{353\}523}, while the other, B, leads to \{110\}hhl\}. Mechanism A cannot operate when the separation of partial dislocations is greater than five times the lattice parameter, in which case the alloy texture is formed. When both mechanisms are operative, as in high stacking fault energy metals, the pure metal texture is formed. Dillamore [99] has questioned the validity of the hypothesis on the grounds that there would in fact be no net reduction in energy due to the dislocation interaction.

Alers and Liu [100] have studied the texture transition in copper due to change in deformation temperature, using Young's modulus methods. They concluded that the texture transition was best explained by the 'mixture' concept (i.e. by varying the fraction of crystals
associated with each of two discrete texture components). This, they stated, was in accordance with the dislocation interaction theory. Recent three dimensional analyses by Bunge and Haessner [11] and Williams [46] have shown that the copper texture is not in fact a simple mixture of two discrete components, but rather a continuous 'tube' of orientations. Since this is contrary to the description of the copper texture claimed to support the dislocation interaction theory, it seems that this theory is not consistent with current experimental evidence.

4.4.6 Recent Proposals

There are probably elements of truth in all of the theories proposed to explain the deformation textures of fcc metals. Experimental evidence now indicates that multiple slip processes are predominant in polycrystalline deformation [85,90,101]. To accommodate an arbitrary shape change, a crystal must have at least five independent modes of shear (see, for example, [77]). Various devices were invoked to overcome this difficulty in models of deformation texture formation, such as the assumption of single slip in the body of the grain, with multiple slip in the grain boundary regions [79,91]. Such assumptions are unrealistic except in coarse grained materials and near free surfaces [101].

Taylor [77] advanced a hypothesis for the choice of five independent slip systems to satisfy a given imposed strain. He considered that the operative combination would be that which satisfied the boundary conditions with the least total shear. Bishop and Hill later showed that Taylor's hypothesis was completely equivalent to their maximum work principle [102,103], both in the general case and in the particular case that Taylor had considered. Chin and Mammel have also shown that a solution to Taylor's analysis is identical with a solution to the Bishop and Hill analysis [104]. This is scarcely surprising
in view of the complete equivalence of the two concepts as demonstrated by Bishop and Hill.

Both Taylor [77] and Bishop [105] analysed the development of fibre textures, but without notable success. Recently, however, a similar analysis has been used by Chin [95] and by Dillamore and Stoloff [96], taking into account as far as possible within the framework of the Taylor/Bishop and Hill analysis the effects of cross slip, latent hardening, and stacking fault formation. Chin et al. [76] have also extended this analysis to the case of mixed slip and twinning, although the value of this analysis is questionable in view of the inhomogeneous nature of the twinning process. Dillamore, Butler, and Green [80] have considered the stability of certain specific orientations under the plane strain conditions expected in sheet rolling. They showed that stable orientations in fcc metals under multiple \{111\}<110> slip conditions are \{110\}<112> and \{4 4 1\}<1 1 1 8> (near \{112\}<111>). These components are both found in the rolling textures of high stacking fault energy metals [80].

4.4.7 Summary

The textures of fcc metals and alloys fall broadly into two types. The 'pure metal' texture is formed by the majority of pure fcc metals during deformation at room temperature, and by alloys during deformation at higher temperatures. The 'alloy' texture is formed by most fcc alloys, by silver during room temperature deformation, and by pure metals when deformed at low enough temperatures or at high strain rates. Stacking fault energy has been identified as an important factor in the texture transition, high stacking fault energy leading to the pure metal texture and low stacking fault energy to the alloy texture.
The principal theories that have been advanced to account for the texture transition are the twinning theory, the cross slip theory, the deformation faulting theory, and the dislocation interaction theory. The twinning theory is the most probable simple explanation of the observed features of the texture transition [80], and twinning is seen to occur under conditions in which the alloy type texture is formed. The importance of cross slip and stacking fault formation cannot be denied, however, since the tendency of a metal to deform by mechanical twinning will be increased when the dislocation mobility is reduced by the formation of stacking faults and the inhibition of cross slip.

Recent theories have tended to incorporate the above theories into the framework of a rigorous analysis of polycrystalline deformation, but a complete analysis of rolling texture formation using such an analysis has not yet been made.
5.1 Introduction

It has become clear that the conflicting theories of the texture transition in fcc metals are due at least in part to the difficulties in the interpretation of conventional texture data. The potentially more powerful three dimensional methods have been used to investigate certain specific fcc textures [11,16,17,46] but a thorough examination of the formation of fcc rolling textures using these methods has not been made. In this chapter the results of an analysis of the development of the rolling textures in commercial copper, Cu - 10 percent Zn (gilding metal) and Cu - 30 percent Zn (brass) at room temperature (~293K) are described.

5.2 X-ray Pole Figures

\{200\}, \{220\}, and \{111\} pole figures were determined for the three materials as described in Chapter 2, at each of 0, 20, 40, 60, 80, 90, and 95 percent rolling reduction. The pole figures are given in Figs. 5.1 to 5.9. The pole figures for the starting materials show that some initial texture was present in each of the materials. Only in the gilding metal was the initial texture particularly significant, being similar to the subsequent rolling texture, but not very well developed.

The pole figures for the deformed materials are consistent with those of previous workers (e.g. [72,82]). Since no essentially new information is revealed, the pole figure data will not be discussed further.
Figure 5.1 (200) pole figures for Copper.

a) Cold rolled 0 percent. Contours at intervals of 0.25
b) Cold rolled 20 percent. Contours at intervals of 0.25
c) Cold rolled 40 percent. Contours at intervals of 0.25
d) Cold rolled 60 percent. Contours at intervals of 0.25
e) Cold rolled 80 percent. Contours at intervals of 0.25
f) Cold rolled 90 percent. Contours at intervals of 0.5
g) Cold rolled 95 percent. Contours at intervals of 0.5
Fig. 5.1b)
Figure 5.2 (220) pole figures for copper.

a) Cold rolled 0 percent. Contours at intervals of 0.25
b) Cold rolled 20 percent. Contours at intervals of 0.25
c) Cold rolled 40 percent. Contours at intervals of 0.5
d) Cold rolled 60 percent. Contours at intervals of 0.5
e) Cold rolled 80 percent. Contours at intervals of 0.5
f) Cold rolled 90 percent. Contours at intervals of
   g) Cold rolled 95 percent. Contours at intervals of
Fig. 5.2b)
Fig. 5.2f)
Figure 5.3 (111) pole figures for copper.

a) Cold rolled 0 percent. Contours at intervals of 0.25
b) Cold rolled 20 percent. Contours at intervals of 0.5
c) Cold rolled 40 percent. Contours at intervals of 0.5
d) Cold rolled 60 percent. Contours at intervals of 0.5
e) Cold rolled 80 percent. Contours at intervals of 1
f) Cold rolled 90 percent. Contours at intervals of 1
g) Cold rolled 95 percent. Contours at intervals of 1
Fig. 5.3b)
Fig. 5.3d)
Fig. 5.3f)

Fig. 5.3g)
Figure 5.4 (200) pole figures for gilding metal.

a) Cold rolled 0 percent. Contours at intervals of 0.25
b) Cold rolled 20 percent. Contours at intervals of 0.25
c) Cold rolled 40 percent. Contours at intervals of 0.25
d) Cold rolled 60 percent. Contours at intervals of 0.25
e) Cold rolled 80 percent. Contours at intervals of 0.5
f) Cold rolled 90 percent. Contours at intervals of 0.5
g) Cold rolled 95 percent. Contours at intervals of 0.5
Fig. 5.4b)

Fig. 5.4c)
Fig. 5.4d)

Fig. 5.e)
**Figure 5.5** (220) pole figures for gilding metal.

a) Cold rolled 0 percent. Contours at intervals of 0.25
b) Cold rolled 20 percent. Contours at intervals of 0.5
c) Cold rolled 40 percent. Contours at intervals of 0.5
d) Cold rolled 60 percent. Contours at intervals of 0.5
e) Cold rolled 80 percent. Contours at intervals of 0.5
f) Cold rolled 90 percent. Contours at intervals of 0.5
g) Cold rolled 95 percent. Contours at intervals of 0.5
Fig. 5.5b)
Fig. 5.5a)
Figure 5.6 (111) pole figures for gilding metal.

a) Cold rolled 0 percent. Contours at intervals of 0.5
b) Cold rolled 20 percent. Contours at intervals of 0.5
c) Cold rolled 40 percent. Contours at intervals of 0.5
d) Cold rolled 60 percent. Contours at intervals of 0.5
e) Cold rolled 80 percent. Contours at intervals of 0.5
f) Cold rolled 90 percent. Contours at intervals of 0.5
g) Cold rolled 95 percent. Contours at intervals of 0.5
Fig. 5.6b)}
Fig. 5.6f)
Figure 5.7 (200) pole figures for brass.

a) Cold rolled 0 percent. Contours at intervals of 0.25
b) Cold rolled 20 percent. Contours at intervals of 0.25
c) Cold rolled 40 percent. Contours at intervals of 0.25
d) Cold rolled 60 percent. Contours at intervals of 0.5
e) Cold rolled 80 percent. Contours at intervals of 0.5
f) Cold rolled 90 percent. Contours at intervals of 0.5
g) Cold rolled 95 percent. Contours at intervals of 0.5
Figure 5.7 (200) pole figures for brass.

a) Cold rolled 0 percent. Contours at intervals of 0.25
b) Cold rolled 20 percent. Contours at intervals of 0.25
c) Cold rolled 40 percent. Contours at intervals of 0.25
d) Cold rolled 60 percent. Contours at intervals of 0.5
e) Cold rolled 80 percent. Contours at intervals of 0.5
f) Cold rolled 90 percent. Contours at intervals of 0.5
g) Cold rolled 95 percent. Contours at intervals of 0.5
Fig. 5.7b)

Fig. 5.7c)
Fig. 5.7d)
Fig. 5.7f)
Figure 5.8 (220) pole figures for brass.

a) Cold rolled 0 percent. Contours at intervals of 0.25
b) Cold rolled 20 percent. Contours at intervals of 0.25
c) Cold rolled 40 percent. Contours at intervals of 0.5
d) Cold rolled 60 percent. Contours at intervals of 0.25
e) Cold rolled 80 percent. Contours at intervals of 0.25
f) Cold rolled 90 percent. Contours at intervals of 0.25
g) Cold rolled 95 percent. Contours at intervals of 0.5
Fig. 5.8b)
Fig. 5.8a)

Fig. 5.8e)
Figure 5.9 (111) pole figures for brass.

a) Cold rolled 0 percent. Contours at intervals of 0.25
b) Cold rolled 20 percent. Contours at intervals of 0.5
c) Cold rolled 40 percent. Contours at intervals of 0.5
d) Cold rolled 60 percent. Contours at intervals of 0.5
e) Cold rolled 80 percent. Contours at intervals of 0.5
f) Cold rolled 90 percent. Contours at intervals of 0.5
g) Cold rolled 95 percent. Contours at intervals of 0.5
Fig. 5.9d)

Fig. e)
Fig. 5.9f)
5.3 Orientation Distribution Function Analysis

The coefficients $W_{lmn}$ of the crystallite orientation distribution function were determined to 20th order as described in Chapter 3. The series truncation error in the pole figures ($\sigma_{\beta}$) and the estimated experimental errors in the pole figures ($\sigma_{\alpha}$) and in the distribution function ($\sigma_{we}$) are given in Table 5.1, normalized so that random corresponds to unity. The only specimen for which series truncation appears to introduce larger errors than those inherent in the measurement is the 95 percent reduced copper. Fig. 5.10 shows the mean absolute values of the $W_{lmn}$, $\bar{W}_{lmn}$, versus order 1, for this specimen. The probable experimental errors $\Delta W_{lmn}$ in these values are also shown. It may be seen that the possible benefit to be gained from increasing the number of terms in the series would be very small.

5.4 Severity of Texture

The development of preferred orientation in the three materials was followed by determining the severity parameter (SP) as described in Chapter 3. This parameter denotes the standard deviation of the orientation distribution from uniformity, and can be used as a basis for comparison of texture development in systems exhibiting different types of texture. Fig. 5.11 shows the variation of SP with reduction for the three materials. A continuous sharpening of the copper texture is apparent, in contrast with the behavior of the gilding metal and brass which show a lower rate of texture development especially above 40 percent reduction.

---

**Table 5.1**

<table>
<thead>
<tr>
<th>a) Copper.</th>
<th>REDUCTION (PERCENT)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ERROR</td>
<td>0  20  40  60  80  90  95</td>
</tr>
<tr>
<td>$\sigma_{\beta}$</td>
<td>0.04  0.07  0.11  0.15  0.19  0.27  0.33</td>
</tr>
<tr>
<td>$\sigma_{\alpha}$</td>
<td>0.08  0.13  0.12  0.15  0.24  0.26  0.28</td>
</tr>
<tr>
<td>$\sigma_{we}$</td>
<td>0.22  0.40  0.38  0.44  0.69  0.79  0.76</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>b) Gilding Metal.</th>
<th>REDUCTION (PERCENT)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ERROR</td>
<td>0  20  40  60  80  90  95</td>
</tr>
<tr>
<td>$\sigma_{\beta}$</td>
<td>0.05  0.09  0.11  0.09  0.10  0.13  0.18</td>
</tr>
<tr>
<td>$\sigma_{\alpha}$</td>
<td>0.09  0.20  0.19  0.11  0.13  0.15  0.25</td>
</tr>
<tr>
<td>$\sigma_{we}$</td>
<td>0.26  0.55  0.53  0.32  0.36  0.44  0.70</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>c) Brass.</th>
<th>REDUCTION (PERCENT)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ERROR</td>
<td>0  20  40  60  80  90  95</td>
</tr>
<tr>
<td>$\sigma_{\beta}$</td>
<td>0.06  0.05  0.08  0.07  0.06  0.10  0.10</td>
</tr>
<tr>
<td>$\sigma_{\alpha}$</td>
<td>0.08  0.12  0.17  0.14  0.11  0.15  0.18</td>
</tr>
<tr>
<td>$\sigma_{we}$</td>
<td>0.25  0.33  0.49  0.40  0.30  0.43  0.50</td>
</tr>
</tbody>
</table>
Figure 5.10. Mean absolute values of the coefficients $W_{\text{mm}}$ of the crystallite orientation distribution function for 95 percent cold rolled copper, indicating the probable errors in the coefficients.

Figure 5.11. Variation of the severity parameter $SP$ with rolling reduction for copper (squares), gilding metal (triangles) and brass (circles).
5.5 Crystallite Orientation Distribution Function

The crystallite orientation distribution function was determined for each specimen at each of 2560 orientations, corresponding to a $6^\circ \times 6^\circ \times 10^\circ$ grid in $\Psi$, $\Theta$, and $\Phi$ in a $90^\circ \times 90^\circ \times 90^\circ$ region of Euler space. Constant $\Phi$ sections of the function are given in Figs. 5.12 to 5.18 for the copper specimens, Figs. 5.19 to 5.25 for the gilding metal, and 5.26 to 5.32 for the brass. Table 5.2 gives a list of the Euler angles corresponding to various ideal orientations (see Chapter 3, section 3.5) which may be used to assist in the interpretation of the distribution functions.
**Table 5.2**

<table>
<thead>
<tr>
<th>Ideal Orientation</th>
<th>Euler Angles</th>
<th>(\theta)</th>
<th>(\phi)</th>
<th>(\psi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>({h k l}) &lt;u v w&gt;</td>
<td></td>
<td>45</td>
<td>0</td>
<td>54.7</td>
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<td>1 1 0 1 1 2</td>
<td></td>
<td>45</td>
<td>90</td>
<td>54.7</td>
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<td></td>
<td>90</td>
<td>45</td>
<td>35.3</td>
</tr>
<tr>
<td>1 1 0 0 0 1</td>
<td>45</td>
<td>0</td>
<td>90</td>
<td></td>
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<td></td>
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<td></td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>45</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>1 1 2 1 1 1</td>
<td>35.3</td>
<td>45</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>65.9</td>
<td>63.4</td>
<td>50.8</td>
<td></td>
</tr>
<tr>
<td>1 2 3 4 1 2</td>
<td>57.7</td>
<td>71.6</td>
<td>75</td>
<td></td>
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<tr>
<td></td>
<td>74.5</td>
<td>56.3</td>
<td>25.1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>36.7</td>
<td>26.6</td>
<td>43.1</td>
<td></td>
</tr>
<tr>
<td>1 0 0 0 0 1</td>
<td>0</td>
<td>(\phi + \psi = 0)</td>
<td>90</td>
<td></td>
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</tr>
<tr>
<td></td>
<td>90</td>
<td>90</td>
<td>90</td>
<td></td>
</tr>
<tr>
<td>1 1 1 1 1 2</td>
<td>54.7</td>
<td>45</td>
<td>0</td>
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<tr>
<td></td>
<td>54.7</td>
<td>45</td>
<td>60</td>
<td></td>
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<tr>
<td>5 5 2 1 1 5</td>
<td>47.1</td>
<td>21.8</td>
<td>74.5</td>
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<td></td>
<td>74.2</td>
<td>45</td>
<td>0</td>
<td></td>
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<tr>
<td>3 5 8 5 2 3</td>
<td>59.7</td>
<td>69.4</td>
<td>68.1</td>
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<td></td>
<td>72.4</td>
<td>58.0</td>
<td>32.6</td>
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<td></td>
<td>36.1</td>
<td>31.0</td>
<td>31.6</td>
<td></td>
</tr>
<tr>
<td>4 4 11 1 1 1 8</td>
<td>27.2</td>
<td>45</td>
<td>0</td>
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<tr>
<td></td>
<td>71.1</td>
<td>70.0</td>
<td>48.4</td>
<td></td>
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</tbody>
</table>

Figure 5.12  Crystallite orientation distribution function for copper, cold rolled 0 percent. Constant \(\phi\) sections, with contours at intervals of 0.25.
Figure 5.13  Crystallite orientation distribution function for copper, cold rolled 20 percent. Constant $\phi$ sections, with contours at intervals of 0.5.

\[ \phi = 0 \]  \[ \phi = 10 \]  \[ \phi = 20 \]  \[ \phi = 30 \]
Figure 5.14  Crystallite orientation distribution function for copper, cold rolled 40 percent. Constant $\phi$ sections, with contours at intervals of 0.5.
Figure 5.15: Crystallite orientation distribution function for copper, cold rolled 60 percent. Constant $\phi$ sections, with contours at intervals of 1.
Figure 5.16  Crystallite orientation distribution function for copper, cold rolled 80 percent. Constant $\phi$ sections, with contours at intervals of 1.
Figure 5.17  Crystallite orientation distribution function for copper, cold rolled 90 percent. Constant $\phi$ sections, with contours at intervals of 1.

$\phi = 0$

$\phi = 10$

$\phi = 20$

$\phi = 30$
Figure 5.18  Crystallite orientation distribution function for copper, cold rolled 95 percent. Constant $\phi$ sections, with contours at intervals of 1.
Figure 5.19  Crystallite orientation distribution function for gilding metal, cold rolled 0 percent. Constant \( \phi \) sections, with contours at intervals of 0.5.
Figure 5.20  Crystallite orientation distribution function for gilding metal, cold rolled 20 percent. Constant $\phi$ sections, with contours at intervals of 0.5.

\[ \theta \]
\[ \psi \]

\[
\begin{array}{ccc}
\phi = 0 & \phi = 10 \\
\phi = 20 & \phi = 30
\end{array}
\]
Figure 5.21 Crystallite orientation distribution function for gilding metal, cold rolled 40 percent. Constant $\phi$ sections, with contours at intervals of 0.5.

\[ \phi = 0 \]
\[ \phi = 10 \]
\[ \phi = 20 \]
\[ \phi = 30 \]
Figure 5.22  Crystallite orientation distribution function for gilding metal, cold rolled 60 percent. Constant $\phi$ sections, with contours at intervals of 0.5.
Figure 5.23  Crystallite orientation distribution function for gilding metal, cold rolled 80 percent. Constant $\phi$ sections, with contours at intervals of 1.
Figure 5.24  Crystallite orientation distribution function for gilding metal, cold rolled 90 percent. Constant $\phi$ sections, with contours at intervals of 1.
\[ \phi = 40 \]

\[ \phi = 50 \]

\[ \phi = 60 \]

\[ \phi = 70 \]

\[ \phi = 80 \]

\[ \phi = 90 \]
Figure 5.25  Crystallite orientation distribution function for gilding metal, cold rolled 95 percent. Constant $\phi$ sections, with contours at intervals of 1.
Figure 5.26  Crystallite orientation distribution function for brass, cold rolled 0 percent. Constant $\phi$ sections, with contours at intervals of 0.25.
Figure 5.27  Crystallite orientation distribution function for brass, cold rolled 20 percent. Constant $\phi$ sections, with contours at intervals of 0.5.
Figure 5.28  Crystallite orientation distribution function for brass, cold rolled 40 percent. Constant φ sections, with contours at intervals of 0.5.
Figure 5.29  Crystallite orientation distribution function for brass, cold rolled 60 percent. Constant $\phi$ sections, with contours at intervals of 0.5.
Figure 5.30  Crystallite orientation distribution function for brass, cold rolled 80 percent. Constant $\phi$ sections, with contours at intervals of 0.5.
Figure 5.31  Crystallite orientation distribution function for brass, cold rolled 90 percent. Constant $\phi$ sections, with contours at intervals of 0.5
Figure 5.32  Crystallite orientation distribution function for brass, cold rolled 95 percent. Constant $\phi$ sections, with contours at intervals of $0.5$. 

\[ \phi = 0 \hspace{1cm} \phi = 10 \hspace{1cm} \phi = 20 \hspace{1cm} \phi = 30 \]
The copper texture (Figs. 5.12 to 5.18) is characterized throughout the range of deformation by a continuous tube of high orientation density, running between \{110\}<112> and (near)\{112\}<111> (in fact the \{441\}<1118> orientation as predicted by Dillamore et al. [80]). Increasing deformation does not alter the basic shape of the texture, but serves to sharpen it.

The texture of the gilding metal (Figs. 5.19 to 5.25) shows a similar initial development to that of copper. At reductions of above 40 percent a depletion of orientations near \{112\}<111> becomes apparent, and very little material is left in this orientation by 95 percent reduction. At the same time as this depletion is evident there is a build up of orientation density in the \{111\}<112>, \{552\}<115>, and \{110\}<001> orientations, none of which are significantly populated in copper at any reduction. It is clear that there is more spread in the gilding metal texture than in the copper texture, supporting the conclusions drawn from Fig. 5.11.

The brass texture (Figs. 5.26 to 5.32) develops along the same lines as that of gilding metal. The depletion of orientations near \{112\}<111> is even more striking, very little material being left in this orientation by 80 percent reduction. The appearance of material in the \{111\}<112>, \{552\}<115> and \{110\}<001> orientations is also apparent, especially after 60 percent reduction. The brass texture is less well developed than that of the gilding metal at all deformations, again supporting the conclusions drawn from the variation of the severity parameter SP with reduction in these metals (Fig. 5.11).

Fig. 5.33 shows the variation of the orientation density with rolling reduction of various ideal orientations. The continuous development of the principal components of the copper texture is clearly
Figure 5.33a. Orientation density of various ideal orientations with rolling reduction for copper.

Figure 5.33b. Orientation density of various ideal orientations with rolling reduction for gilding metal.
Figure 5.33c. Orientation density of various ideal orientations with rolling reduction for brass.
seen in Fig. 5.33a. The texture transition occurring at about 60 percent reduction in gilding metal (Fig. 5.33b) and brass (Fig. 5.33c) is shown by the reduction of the \{112\}<111> orientation density, together with the increase in the \{552\}<115> component. A difference between the gilding metal and brass is seen in the \{123\}<412> component, which continues to develop in gilding metal, but remains roughly static above 60 percent reduction in brass.

The density of orientations having a [110] transverse direction (\(\psi = 0, \phi = 45\) degrees) is shown in Fig. 5.34. Dillamore et al. [80] have shown that the choice of \{111\}<110> slip systems for these orientations is unique, and that the slip rotations for crystals in these orientations are also uniquely determined. Once again the difference in behaviour of the three materials is clearly apparent.

The development of the range of orientations corresponding to the copper orientation tube is shown in Fig. 5.35 for the three materials. The initial build up, and subsequent depletion, of orientations at the \{4 4 1\}<11 11 8> end of the orientation tube is seen in gilding metal and brass, while the overall shape for the copper is maintained to 95 percent reduction. The change in relative prominence of the \{110\}<112> and \{4 4 1\}<11 11 8> orientations in the copper between 90 and 95 percent reduction, although not significant within the accuracy of the results (see Table 5.1) is consistent with the findings of Hu et al. [72] who attribute it to dynamic recovery.

The volume fraction (percent) of crystallites oriented within 10 degrees of the \{110\}<112>, \{4 4 1\}<11 11 8>, and \{552\}<115> orientations are given in Table 5.3. The same trend is seen as in Fig. 5.33, but it shows that the amount of material associated with the
Figure 5.34a. Illustrating the variation of orientation density with rolling reduction for orientations having a <110> transverse direction ($\psi = 0, \phi = 45^\circ$) in copper.

Figure 5.34b. Illustrating the variation of orientation density with rolling reduction for orientations having a <110> transverse direction ($\psi = 0, \phi = 45^\circ$) in gilding metal.
Figure 5.34c. Illustrating the variation of orientation density with rolling reduction for orientations having a <110> transverse direction ($\psi = 0, \phi = 45^\circ$) in brass.

Figure 5.35a. Illustrating the variation of orientation density with rolling reduction for orientations between {110}<112> and {111}<110> in copper.
Figure 5.35b. Illustrating the variation of orientation density with rolling reduction for orientations between \{110\}<112> and \{441\}<1118> in gilding metal.

Figure 5.35c. Illustrating the variation of orientation density with rolling reduction for orientations between \{110\}<112> and \{441\}<1118> in brass.
### Table 5.3

**Fraction (%) of Crystals within 10° of the Given Ideal Orientation**

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<thead>
<tr>
<th>ORIENTATION</th>
<th>REDUCTION (PERCENT)</th>
</tr>
</thead>
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<tr>
<td>{1 1 0} {1 1 2}</td>
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</tr>
<tr>
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<tr>
<td>{4 4 1} {1 1 6}</td>
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<table>
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<th>REDUCTION (PERCENT)</th>
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</thead>
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<td>{1 1 0} {1 1 2}</td>
<td>4.7</td>
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<tr>
<td>{5 5 2} {1 1 5}</td>
<td>1.1</td>
</tr>
<tr>
<td>{4 4 1} {1 1 6}</td>
<td>3.0</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>ORIENTATION</th>
<th>REDUCTION (PERCENT)</th>
</tr>
</thead>
<tbody>
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</tr>
<tr>
<td>{1 1 0} {1 1 2}</td>
<td>3.5</td>
</tr>
<tr>
<td>{5 5 2} {1 1 5}</td>
<td>1.3</td>
</tr>
<tr>
<td>{4 4 1} {1 1 6}</td>
<td>1.9</td>
</tr>
</tbody>
</table>
orientation at a given rolling reduction is more nearly equal in the three materials than Fig. 5.33 suggests. This is due to the greater orientation spread evident in the gilding metal and brass textures. The correlation of the disappearance of material from the region of the \(\{4\ 4\ 1\}\<11\ 1\ 1\>\) orientation with the appearance of material in the region of the \(\{552\}<115>\) orientation is quite apparent. It is significant that so little material is associated with the principal texture components, in agreement with the findings of Williams [46] and Kallend and Davies [56]. This emphasises the inadequate description of textures given by ideal orientations.

5.6 Discussion

5.6.1 Pure Metal Texture

The development of the copper texture is seen to be a continuous process over the range of deformation investigated. The result of increasing deformation is to sharpen the texture without affecting the overall shape. The texture is best described as a continuous range of orientations between \(\{110\}<112>\) and \(\{4\ 4\ 1\}\<11\ 1\ 1\>\). This is not consistent with the description of the copper texture as two limited fibre textures, due to Wassermann [83], nor with the description of Liu [98] who considers it to be composed of two discrete components \(\{110\}<112>\) and \(\{358\}<523>\).

The original cross slip theory of Dillamore and Roberts [79] predicted a copper texture at high deformations which is consistent with the present results. This theory does not, however, predict the development of the copper texture that was observed. In the light of the analysis of Dillamore and Roberts it seems that cross slip is active from the initial stages of the deformation process, leading to
homogeneous deformation, which in turn will promote the sharp final texture.

Dillamore et al. [80] have shown that both \(\{441\}<1118>\) and \(\{110\}<112>\) orientations are stable under multiple slip conditions. Dillamore [97] considers that these components form the extremes of a range of orientations that would be obtained under polyslip conditions. The present results are consistent with this hypothesis.

5.6.2 Alloy Texture

The textures of both gilding metal and brass exhibit an initial development of a range of orientations similar to that seen in copper, but at reductions of above about 40 percent there is a marked depletion of orientations at the \(\{441\}<1118>\) end of the range. At the same time an increase in the density of orientations between \(\{111\}<112>\) and \(\{110\}<001>\), with considerable spread, is observed. The textures of both gilding metal and brass are less severe than that of copper.

The observed features of the textures of gilding metal and brass are not consistent with either the simple cross slip theory [79] (see Chapter 4, section 4.4.3), or with the dislocation interaction theory of Liu [98] (see Chapter 4, section 4.4.5). Dillamore et al. [80] have shown that multiple slip processes cannot lead to the build up of material in the range \(\{111\}<112>\) to \(\{552\}<115>\). This can, however, be explained if mechanical twinning occurs in crystals whose orientations lie at the \(\{112\}<111>\) end of the range of orientations which is formed at low deformations. The effect of mechanical twinning would be mirror imaging in the twin plane, and a rotation due to the shear in a \(<112>\) direction. For example, a crystal with a \(\{112\}<111>\) orientation would twin to \(\{552\}<115>\), and the shear rotation would carry it towards
Subsequent slip deformation would then take it towards \{113\}<001> [80] (evidence of slip in micro-twins has been obtained by Hu et al. [72]). All of these orientations were found to be significantly populated at higher deformations in gilding metal and brass, but not in copper. The observed twins in fcc alloys have been thin micro-twins, distributed throughout the crystal [72,85]. Consequently the untwinned portion of the crystal would also be subject to a rotation due to a \{112\} shear. This would take it towards \{111\}<112>. The same effect would be produced by stacking fault formation, which also leads to a \{112\} shear [72], but this mechanism could not account for the appearance of material in orientations around \{552\}<115>.

The increased spread apparent in the textures of gilding metal and brass as compared with that of copper is probably due to two sources. The tendency to form deformation bands (independently deforming regions within a grain) is expected to increase as the stacking fault energy is lowered [97]. This would result in an increased spread about the mean orientation. Further spread would be caused by mechanical twinning, since the operation of two different deformation mechanisms (i.e. slip and twinning), each producing different crystal reorientations, would tend to produce a dynamic equilibrium between the effects due to each.

5.7 Summary

The crystallite orientation distribution function has been determined for cold rolled copper, gilding metal, and brass at cold reductions of 0, 20, 40, 60, 80, 90, and 95 percent. The copper texture exhibits a steady development, and contains components which have been shown to be stable during multiple slip processes (i.e. \{110\}<112> and \{4 4 11\}<11 11 8>). The textures of gilding metal and brass both show a
similar initial development to that of copper, but a transition occurs above a reduction of about 40 percent, indicating that an additional deformation mode is activated at higher reductions. The features of the transition are consistent with those expected if the additional deformation mode were mechanical twinning.
6.1 Introduction

Numerous theories have been advanced to explain the existence of the two types of rolling texture in fcc metals and alloys. Comprehensive analyses of the predicted crystal rotations leading to fibre textures have been made by several authors [77,95,96,105], but for the most part the theories of rolling texture formation have been limited to predicting stable end orientations, or following the rotations of crystals with specific orientations. Jeffers [91,106], however, has predicted pole figures based on his theory of the fcc texture transition. Although the assumptions that he has made are open to question (see Chapter 4), the comparison of predicted textures with those determined experimentally is clearly the most satisfactory test for any theory of texture development. This chapter describes a simulation of rolling texture development, taking account of \{11\}<110> multiple slip. The effects of mechanical twinning on the predicted textures are also considered.

6.2 Polycrystalline Deformation

Theories of polycrystalline deformation fall basically into two classes, those which achieve stress equilibrium, and those which achieve strain compatibility. Theories of the former type (e.g. [107]) are unrealistic except for coarse grained materials at small deformations (<0.05 percent shear strain [108]), and available evidence [101,108,109] indicates that strain compatibility is of overriding importance at the deformations typical of metal working processes.
Taylor [77] suggested a method for the choice of the set of five independent slip systems needed to maintain strain continuity. Taylor considered that the active set would be that which would satisfy the imposed strain with the minimum plastic work. This hypothesis was later shown by Bishop and Hill [102,103] to be equivalent to their maximum work principle. Bishop and Hill also showed that Taylor's assumption of homogeneous strain throughout the polycrystal was unnecessary, and Kocks [108] states that considerable deviations from homogeneity can be tolerated without significantly affecting the results. Bishop and Hill [103] showed that in order to sustain plastic flow in a region of a polycrystal, the critical shear stress should be attained on at least five independent systems, without being exceeded on any system. This could only be achieved by a finite number of stress states. For \{111\}<110> slip in a fcc lattice, assuming that all slip systems are equally hardened, Bishop and Hill showed that there are five essentially different types of stress state which fulfill the yield criterion. These stress states are denoted types (i), (ii), (iii), (iv), and (v). Because of crystal symmetry there are 6 members in each of (i) and (ii), 12 in (iii), 24 in (iv), and 8 in (v). The critical shear stress is attained in 8 slip systems for (i), (ii), and (iii), and in 6 slip systems for (iv) and (v). The active stress state for any given imposed strain is that which does the maximum plastic work in that strain [102].

Although strain compatibility is achieved by this theory, it is clear that continuity of stress cannot be maintained by a number of volume elements each subject to a uniform stress. Bishop and Hill [102] state that this objection can be removed as the size of the element considered tends to zero. Kocks [108] has also considered the problem of stress equilibrium. He considers that any necessary adjustment of stresses can be made by elastic distortions, the strains being
negligible with respect to the plastic ones for all reasonable stress adjustments. This, however, leads to a violation of the yield condition [109].

Bishop [110] has listed the \{111\}<110> stress states and illustrated the determination of the shear on each slip system necessary to conform with the imposed strain. Since either six or eight systems are equally stressed, whereas only five are required in order to satisfy an arbitrary imposed strain, the shears are not in general uniquely determined, but can vary within certain limits (although the shears are uniquely determined for certain lattice orientations under a given imposed strain [80]). Dillamore and Stoloff [96] have listed the active slip systems for one example of each of the five types of stress state. They show that two <110> directions are activated in each active slip plane in all of the stress states.

The effect of material properties on the choice of shears within the limits imposed by the maximum work principle has been considered by Bishop [105], Chin [95], and Dillamore and Stoloff [96]. Bishop suggested that the phenomenon of overshoot, observed in low stacking fault energy materials, would show up in multiple slip by maximising the shear on the most favoured slip system. No tendency to overshoot would favour combinations in which the total shear was most evenly distributed between the active systems.

The correlation of the texture transition with stacking fault energy led Chin [95] and Dillamore and Stoloff [96] to consider the effects of dislocation dissociation on the choice of shears. Chin considered that under conditions leading to extended dislocations, activity on slip systems with a common slip plane would harden the intersecting planes with the result that slip on that coplanar pair
would be maximised. When dislocations were not extended, slip on cross related systems (colinear systems) would be favoured. In fact only in stress states of type (iv) (Bishop and Hill's notation [103]) is the total activity of coplanar pairs a variable, since the shears on coplanar systems are linearly related in all other stress states. Similarly, the activities of colinear pairs are only a variable in stress states of type (iii). The result of this is that the fibre textures predicted by these two mechanisms are virtually identical [95].

Dillamore and Stoloff [96] have considered the effect of the stress state on the Shockley partials formed by the dissociation of \{111\}<110> dislocations. Since two <110> directions are equally stressed in all active slip planes, the maximum shear stress in the \{111\} plane must be along <121>, and will either extend or constrict the slip dislocations. Dislocations of both active systems in a given slip plane are extended or constricted together. Dillamore and Stoloff have listed the extended and constricted systems for one example of each type of stress state. They consider that the effect of a low stacking fault energy is to cause the maximization of shears parallel to a plane on which dislocations are extended, on the grounds that stacking faults form an effective forest inhibiting intersecting slip. This principle can be applied in stress states of type (ii), (iii), and (iv), although in each of these there are two planes on which dislocations are extended, and maximization of the shears on one tends to minimize the shears on the other. Dillamore [97] considers that equally probable but mutually exclusive shear combinations are equally likely to occur, and that this would increase the tendency to deformation banding.

The effect of high stacking fault energy is considered to favour those constricted systems in cross relationship. Only stress states of
type (iii) produce any clear tendency for this to occur, since the shear on cross related systems is not a variable in states (i), (ii), (iv), and (v), and the total shear on constricted systems is not a variable in states of type (i), (ii), and (v).

Dillamore [97] has emphasized that the stress states listed by Bishop [110] are only strictly applicable to situations where all slip systems are equally hardened. Consequently, any tendency to favour one or more systems because of the assumed effects of material properties will in fact invalidate these stress states. It is not thought that this will significantly affect the results as long as extremes of behaviour such as the complete separation of partial dislocations leading to \{111\} <112> slip, or at the other extreme, pencil glide, are avoided.

6.3 Crystal Rotations

The crystal displacement \( u_i \) at a position \( x_i \) may be determined from the relation [110]

\[
u_i = \sum_{\alpha, \beta, j} d\gamma_{\alpha \beta} n_j \alpha x_j l_i \alpha \beta
\]

where \( d\gamma_{\alpha \beta} \) is the shear on the plane \( \alpha \), normal \( n_\alpha \), in the slip direction \( \beta \), specified by the direction cosines \( l_i^{\alpha \beta} \) \((i = 1, 2, 3)\). The displacement matrix is given by,

\[
\frac{du_i}{d\alpha_j} = \sum_{\alpha \beta j} d\gamma_{\alpha \beta} n_j^{\alpha \beta} l_i^{\alpha \beta} \tag{6.1}
\]

the rotation, \( \zeta \), of the crystal relative to the principal axes of strain increment is given by [105]:

\[
\zeta = -\frac{1}{2} \text{curl} \ u \tag{6.2}
\]

and the axis of rotation has direction cosines [80]:
\[ a_i = \frac{\sum d \xi_j}{(\sum d \xi_j)^{1/2}} \quad (i = 1,2,3) \]

The crystal orientation following the rotation is given by the congruent transformation:

\[ T' = [\tilde{A} R A] T \quad (6.3) \]

where \( T \) and \( T' \) are the initial and final orientation matrices relating the crystal axes with the specimen axes, \( A \) is a matrix relating the axis of rotation with the crystal axes

\[
A = \begin{pmatrix}
\cos \beta \cos \alpha & \cos \beta \sin \alpha & -\sin \beta \\
-\sin \alpha & \cos \alpha & 0 \\
\sin \beta \cos \alpha & \sin \beta \sin \alpha & \cos \beta
\end{pmatrix}
\]

where \( \alpha, \beta \) are the azimuthal and polar coordinates of the rotation axis,

\[
R = \begin{pmatrix}
\cos \xi & \sin \xi & 0 \\
-\sin \xi & \cos \xi & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

where \( \xi \) is the rotation about the axis.

6.4 Computer Simulation of FCC Rolling Texture

6.4.1 Operation of Program

The computer simulation of the formation of rolling texture was performed on 406 hypothetical crystals, distributed uniformly in the region of Euler space \( 0 \leq \psi \leq 90 \), \( 0 \leq \theta \leq 90 \), \( 0 \leq \phi \leq 90 \). Each crystal was subject to a simulated rolling strain increment, relative to the specimen axes, of:
The strain relative to the crystal axes was computed, and the work done in the strain by each of the Bishop and Hill stress states for \( \{111\}<110> \) slip was determined. The operative state was that for which the work done was a maximum. The shears in the active slip systems were computed; these specified the resultant crystal rotation. The new crystal orientation was found from equation (6.3), and the process was repeated until the total simulated rolling reduction received by each crystal was 80 percent. At 40 percent, 60 percent, and 80 percent reduction the orientations of the crystals were plotted in constant sections of Euler space, at 10° intervals in \( \beta \) between 0 and 90°. All crystals within 5° of the section were plotted on the section, those on or above the section were plotted as a short vertical line, and those below the section as a short horizontal line.

6.4.2 Choice of Shears in Operative Slip Systems

Two methods were used to allocate shears on the operative slip systems within the limits imposed by the maximum work principle, in an attempt to simulate the behaviour of high stacking fault energy and low stacking fault energy materials respectively. To simulate high stacking fault energy behaviour the activity on cross related, constricted pairs of slip systems was maximized in stress states of type (iii). In all other stress states the shears were chosen at random within the permitted limits, since in these states there is no clear indication of the effect of high stacking fault energy. The effect of this random choice is that after a number of strain increments the total shear is fairly evenly distributed among the active slip systems.
The effect of low stacking fault energy behaviour was simulated by choosing the shears to maximise the activity on an extended plane in stress states of types (ii), (iii), and (iv). The choice of which particular extended plane was chosen was made at random (the high incidence of deformation banding in low stacking fault energy materials indicates that no consistent choice of shears is made). In states of type (i) and (v), where activity on extended planes is not a variable, the activity on one system, chosen at random, was maximized.

6.4.3 Effect of Mechanical Twinning

In order to gain some idea of the effect of mechanical twinning on deformation texture formation, the possibility of twin formation was incorporated into the computer program. Chin et al. [76] have incorporated the possibility of mixed slip and twinning into the Taylor analysis, and have shown that it can satisfactorily explain some of the observed features of the deformation of single crystals of Co - 8 percent Fe, a very low stacking fault energy fcc alloy. The value of an approach based on a principle of near homogeneous deformation, and in which no allowance can be made for twin - twin and twin - slip interactions, is questionable. There is some doubt as to the existence of a critical stress for twinning [111] which is assumed to exist in this analysis, and it is also very difficult to allow for the continuous change in glide stress due to hardening of the lattice. For these reasons it was decided to adopt a very much simpler, albeit arbitrary, approach.

At each step in the deformation above a strain of 0.3 (~25 percent reduction) each crystal was given a chance to twin. The probability of twinning was weighted by a 'twinning parameter', which was determined by the extent to which twinning on the most favoured
\{11\}<112\> twin system could accommodate the imposed strain, and also by the difficulty of maintaining multiple slip in the crystal (the Taylor factor \[101\]). Of the orientations likely to be produced by slip processes (see e.g. \[79,80,81,83\]) these criteria indicate that twinning is most likely at orientations near \{11\}<111\>, and very unlikely at orientations near \{11\}<112\>. The analysis of Chin et al. \[76\] predicts a similar behaviour, and such assumed behaviour forms the basis of Wassermann's twinning theory \[83\]. Deformation twinning has not been observed in \{11\}<112\> crystals, even of very low stacking fault energy alloys \[76\]. Furthermore, twinning is scarcely observed at all in the room temperature deformation of copper crystals, even at the favoured orientation \{11\}<111\> \[72\]. In a typical material exhibiting the 'alloy' texture (e.g. \(\alpha\)-brass) the behaviour is probably intermediate, with twinning only occurring at the \{11\}<111\> end of the range of orientations. In this simulation the twinning probability was made linearly dependent on the 'twinning parameter', in such a way that the twinning probability varied from unity at the favoured \{11\}<111\> orientation to zero at \{123\}<412\>* (an orientation intermediate between \{11\}<111\> and \{11\}<112\>). In the absence of a satisfactory theory of polycrystalline twinning behaviour the use of an arbitrary criterion such as that described seems unavoidable.

* The effect of varying the value of the twinning parameter corresponding to zero twinning probability was investigated. It was not found to affect the results significantly, except to increase the amount of scatter in the predicted orientations as more orientations were allowed to twin, and vice versa.
The crystals were considered in pairs, and when a twinning event occurred one crystal underwent the twinning reorientation, and both were subject to a shear reorientation (i.e. a rotation due to the shear on \{11\{1\}<112\}). The effect of this was to simulate a crystal in which 50 percent of the volume had twinned (Heye and Wassermann [112] observed that the typical volume fraction of a crystal that twinned was 50 percent). Up to three twinning events were permitted in any crystal. After a twinning event, subsequent slip deformation was allowed (Hu et al. [72] observed that slip took place within micro-twins in Cu-4 percent Al). All slip deformation took place within the framework of the Bishop and Hill maximum work principle, with the choice of shears made as described in section 6.4.2 for low stacking fault energy materials.

6.5 Results

6.5.1 Textures Resulting from Multiple Slip

The predicted textures resulting from multiple slip processes are given in Figs. 6.1 to 6.6. The crystal end orientations for 40 percent, 60 percent, and 80 percent reduction assuming conditions favouring cross slip (the 'cross slip' texture) are given in Figs. 6.1, 6.2, and 6.3, and those for conditions favouring dislocation dissociation (the 'extended' texture) in Figs. 6.4, 6.5, and 6.6. The crystal orientations clearly tend towards the orientation tube as observed in copper at all three reductions, and comparison with Figs. 5.14, 5.15, and 5.16 shows that the predicted cross slip texture agrees well with the experimentally determined copper texture. At 40 percent reduction there is slightly more scatter in the extended texture than in the cross slip texture, and slightly fewer crystals at the \{4\{4\<1\}1\}<11\,1\,8\> end of the orientation tube. The difference is so small, however, that it is probably not significant in view of the
limited number of crystals considered in the analysis (i.e. 406). At higher reductions there is very little to choose between the cross slip texture and the extended texture, both of which give good agreement with the experimentally determined copper texture. The extended texture is clearly incompatible with the experimentally determined textures of gilding metal and brass at 60 percent and 80 percent reductions (Figs. 5.22, 5.23, 5.29, 5.30). The \{111\} pole figure corresponding to the cross slip texture at 80 percent reduction is given in Fig. 6.10, together with the measured \{111\} pole figure for 80 percent cold rolled copper.

6.5.2 Predicted Textures when Twinning Permitted

The predicted crystal orientations after 40 percent, 60 percent, and 80 percent reduction when twinning is permitted as a possible deformation mode (the 'twinning' texture) are given in Figs. 6.7, 6.8, and 6.9. The expected reduction in the number of crystals at the \{112\}<111> end of the orientation range is apparent, together with a build up of crystals near the \{552\}<115> orientation. Comparison with the experimentally determined textures of gilding metal and brass (Figs. 5.21 to 5.23 and Figs. 5.28 to 5.30) shows that the predicted textures are consistent with the observed features of these textures. The twinning texture shows considerably more scatter than the cross slip texture or the extended texture. The \{111\} pole figure corresponding to the twinning texture at 80 percent reduction is given in Fig. 6.11, together with the measured \{111\} pole figure for 80 percent cold rolled gilding metal.

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Figure 6.1  Predicted orientation distribution for the 'cross slip' texture at 40 percent reduction. Constant $\phi$ sections.
Figure 6.2  Predicted orientation distribution for the 'cross slip' texture at 60 percent reduction. Constant $\phi$ sections.
Figure 6.3  Predicted orientation distribution for the 'cross slip' texture at 80 percent reduction. Constant $\phi$ sections.
Figure 6.4  Predicted orientation distribution for the 'extended' texture at 40 percent reduction. Constant $\phi$ sections.
Figure 6.5 Predicted orientation distribution for the 'extended' texture at 60 percent reduction. Constant $\phi$ sections.
Figure 6.6  Predicted orientation distribution for the 'extended' texture at 80 percent reduction. Constant $\phi$ sections.
Figure 6.7 Predicted orientation distribution for the 'twinning' texture at 40 percent reduction. Constant $\phi$ sections.
Figure 6.8 Predicted orientation distribution for the 'twinning' texture at 60 percent reduction. Constant $\phi$ sections.
Figure 6.9  Predicted orientation distribution for the 'twinning' texture at 80 percent reduction. Constant $\phi$ sections.
Figure 6.10  Predicted (111) pole figure for the 'cross slip' texture at 80 percent reduction, with the (111) pole figure for 80 percent cold rolled copper superimposed.

Figure 6.11  Predicted (111) pole figure for the 'twinning' texture at 80 percent reduction, with the (111) pole figure for 80 percent cold rolled gilding metal superimposed.
The observed features of the development of the rolling texture in copper are consistent with the predictions of an analysis based on the assumption that the dominant deformation process is multiple \{111\}<110> slip. The development of rolling texture in gilding metal and brass, however, cannot be explained by multiple slip processes alone. If mechanical twinning is considered as an additional deformation mode the predicted textures agree satisfactorily with the experimental data for these alloys.

The effect of stacking fault energy on the behaviour of slip dislocations has been considered within the framework of the maximum work principle, and textures have been predicted based on the probable effects of both high and low stacking fault energy. The differences between the predicted textures was very slight, and both were consistent with the experimentally determined copper texture. Similar results were found by Chin [95] and Dillamore and Stoloff [96] who found that the predicted fibre textures arising from \{111\}<110> multiple slip were only marginally altered by assumptions made about dislocation behaviour. This is to be expected as orientation space is divided into regions in which particular stress states are active, and the boundaries between these regions correspond to orientations with uniquely determined slip rotations. Consequently a basic pattern is imposed on the deformation texture which is independent of material variables [97].

In the copper - zinc alloys investigated any small texture variation due to the possible influence of stacking fault energy on the choice of shears in the active slip systems would be impossible to detect experimentally since they would be swamped by the gross reorientations due to mechanical twinning. Dillamore and Stoloff [96]
have investigated the rolling texture of ordered Cu₃Au, rolled 95 percent. This material behaves as if it had a low stacking fault energy except that twinning is not a possible deformation mode. The \{111\} pole figure for this material is remarkably similar to that of 50 percent cold rolled copper (Fig. 47a of [72]) and to that of 60 percent cold rolled copper (Fig. 5.3d, Chapter 5). This indicates that the primary effect of reducing the stacking fault energy in the absence of mechanical twinning is to increase the amount of spread in the texture rather than to alter the basic distribution of orientations, since a low stacking fault energy is conducive to the formation of deformation bands.

The effect of the formation of deformation bands has not been considered explicitly in the simulation of texture development described in this chapter. Chin [95] and Wonsiewicz and Chin [78] have shown that two types of deformation band observed in fcc metals can be explained in terms of the Taylor/Bishop and Hill analysis. Type 1 deformation bands are formed when a different permissible combination of slip systems operates in each of several regions of a crystal, and type 2 deformation bands form if the the work done by slip within the bands is less than that required for homogeneous deformation, while the net strain matches that for the overall deformation. Provided that each region is treated as a separate, homogeneously deforming body the analysis remains valid. The effect of deformation banding on the simulated textures described in this chapter would be to increase the spread in the crystal end orientations without altering the overall distribution.

A further factor increasing the orientation spread is the occurrence of mechanical twinning, as seen in Figs. 6.7 to 6.9. This, taken with deformation banding, would explain the increase in the
severity of the texture at any given reduction in going from brass through gilding metal to copper. It would also explain why the \{111\} pole figure of Cu$_3$Au [95], in which deformation bands but not twins occur, is less sharp than that of copper, and sharper than that of Cu-30 percent Zn at the same reduction (see e.g. [72], and Figs. 5.3g, and 5.9g, Chapter 5).

The fcc texture transition is brought about not only by alloying, but also by lowering the deformation temperature or increasing the deformation rate (see Chapter 4). In the absence of other effects, neither of these processes should have any significant influence on the frequency of mechanical twinning, which is seen to be the mechanism giving rise to the transition. However, since the movement of dislocations during the multiple slip processes is to a large extent dependent on their ability to negotiate a highly distorted lattice, the ease with which cross slip and dislocation intersection can occur will be of the utmost importance. Both of these processes are thermally activated, the activation energy being reduced when a stress is applied in the correct sense [93]. Consequently a reduction in temperature or an increase in the deformation rate will both increase the general level of stress in the crystal needed to maintain deformation by slip, and this increase in stress will be responsible for the onset of mechanical twinning. The effect of a reduction in stacking fault energy would be twofold, as not only does the separation of partial dislocations increase (the separation is proportional to $G\beta/\gamma$) which increases the activation energy for cross slip and dislocation intersection (jog formation), but the stacking faults formed by the separation of the partials will also serve as nuclei for twins [93]. It would seem, therefore, that the texture transition in fcc metals is due to the change in the behaviour of slip dislocations with material and process...
variables, but that the transition is brought about predominantly through the agency of mechanical twinning.
PART III

CORRELATION OF TEXTURE AND PROPERTIES

IN CUBIC METALS
7.1 Introduction

Any property which exhibits anisotropy in single crystals of a material will in general be anisotropic in a textured aggregate of that material. Magnetic, plastic, and elastic properties are those in which anisotropy has the greatest practical importance, and a great deal of the literature has been devoted to the effects of texture on these properties (see e.g. [1,31,113,114]). From a metallurgical viewpoint the elastic and plastic properties are of the greatest interest, and some of the existing information relating these with texture is reviewed in this chapter.

7.2 Elastic Anisotropy

7.2.1 Single Crystals

The relationship between elastic stresses and strains in a single crystal is given by the generalized Hooke's Law [115],

\[ \varepsilon_{ij} = \sum_{k,l} S_{ijkl} \sigma_{kl} \quad i,j,k,l = 1,2,3 \]

where \( S_{ijkl} \) are elements of the elastic compliance tensor. The reciprocal relation is:

\[ \sigma_{ij} = \sum_{k,l} c_{ijkl} \varepsilon_{kl} \]

Here \( c_{ijkl} \) are elements of the elastic modulus tensor. The compliance and modulus tensors are usually represented in two dimensional form as \( 9 \times 9 \) matrices [115]. The elements of these tensors are not all independent since restrictions are imposed by the symmetry of the
crystal class to which the material belongs, and by the symmetry of the stress and strain tensors. For cubic crystals only three of the elements are independent, \( s_{11} \), \( s_{12} \), and \( s_{44} \) (along with the corresponding elements in the modulus tensor)[115].

If a specimen is prepared from a crystal of cubic material so that the direction cosines of the specimen axis with respect to the crystal axes are \( l_1, l_2, l_3 \), then the Young's modulus of the specimen is given by [115]

\[
\frac{1}{E} = s_{11} - 2(s_{11} - s_{12} - 0.5 s_{44}) \gamma
\]

where \( \gamma = l_1^2 l_2^2 + l_2^2 l_3^2 + l_3^2 l_1^2 \).

The crystal will be elastically anisotropic if

\[ s_{11} - s_{12} - 0.5 s_{44} \neq 0 \]

This condition is fulfilled by the majority of cubic metals, exceptions being aluminium and tungsten.

7.2.2 Polycrystals

The elastic properties of a polycrystalline aggregate are clearly dependent on the elastic properties of the constituent crystals (although it does not necessarily follow that a knowledge of the single crystal properties is sufficient to define the properties of the aggregate). Methods for determining the elastic properties of polycrystals have been proposed by Voigt [24], who assumed that the strain was uniform throughout the specimen, and by Reuss [25], who assumed uniform stress. Hill [26] showed that these two assumptions lead to an upper and lower bound, respectively, for the true polycrystal data. He proposed taking the mean value of the Voigt and Reuss averages as a better approximation.
Exact theories have been developed (e.g. [27,28]) which take into account the boundary conditions of both stress and strain, but these are so complex that they have found little application.

7.2.3 Correlation with Crystallographic Texture

Equation (7.1) forms a basis for the correlation of Young's modulus with crystallographic texture. Weerts [18] assumed that the quantity \(1/E\) was additive for each orientation present, and computed the variation in Young's modulus in rolled and recrystallized sheets. The textures for these computations were assumed to be \(\{110\}<112>\) and \(\{112\}<111>\) in equal amounts for the rolled sheets, and \(\{001\}<100>\) for the recrystallized material. The results did not agree very well with the measured values for the rolled sheet, but satisfactory agreement was achieved with the recrystallized sheet. Similar methods have recently been used to supplement pole figure data in assigning ideal orientations by Alers and Liu [19] and Hoddinott and Davies [20].

Pursey and Cox [22] showed that the orientation dependent part of equation (7.1) could be described exactly by a fourth order spherical harmonic function. They showed for the case of fibre textures that if the inverse pole figure is similarly expanded into a series of spherical harmonics, then only the fourth order term can contribute to elastic anisotropy because of the orthogonality of these functions (see Chapter 3). Pursey and Cox did not analyse any experimental data, presumably because of the difficulties in obtaining inverse pole figures at that time (1953).

An extension of the approach of Pursey and Cox has been used by Bunge and co-workers [23,116,117] and by Kallend and Davies [118] in order to correlate the anisotropy of Young's modulus with texture in
rolled sheets. This is described in Chapter 8.

7.3 Plastic Properties

7.3.1 Single Crystals

It has long been established that the dominant feature in the plastic deformation of metals at sub-diffusive temperatures is glide on certain crystallographic planes in certain crystallographic directions. Such a combination of glide plane and direction comprises a slip system, and the particular slip system which operates is that on which the resolved shear stress is a maximum [119]. The yield strength of a plastic crystal depends on the orientation relationship represented in the Schmid Law [120]

\[ \tau = \frac{\tau}{\cos \phi \cos \lambda} \]

where \( \tau \) is the applied stress, \( \tau \) the critical resolved shear stress for glide on the active slip system, and \( \phi \) and \( \lambda \) are respectively the angles of the slip plane normal and the slip direction from the applied stress. It is clear that the plastic behaviour of a single crystal will be anisotropic.

7.3.2 Polycrystals

Grains in a polycrystal are generally subject to more complex boundary conditions of stress and strain than single crystals in a tensile test, and it is not usually possible to infer the behaviour of a polycrystal from the known behaviour of its constituent grains when free from constraint [101]. There have been many attempts to correlate single crystal behaviour with that of polycrystals (e.g. [77,102,103,107,108]), and Kocks [101] has recently reviewed the principal theories. Recent developments tend to support the theories which achieve strain compatibility (see Chapter 6, section 6.2), and the solution due to
Taylor [77], along with the equivalent approach of Bishop and Hill [102,103], are considered to be good approximations at strains greater than about 1 percent [108,109]. Both of these solutions predict the work done in a given imposed strain in terms of the critical shear stresses on the individual slip systems. Kocks [108] has pointed out that these critical stresses, obtained from experiments on single crystals, should be determined under multiple slip conditions in order to be applicable to polycrystals. The experimental results of Hosford [121] and of Chin et al. [122] have validated the Taylor/Bishop and Hill analysis, although Mayer and Backofen [123] have found considerable deviations from it in low stacking fault energy materials. This could well be due to their experimental technique which did not eliminate shear strains, although these were assumed to be absent in their analysis. Chin et al. [122] showed that the predicted results were quite sensitive to shear strains.

7.3.3 Practical Importance of Plastic Anisotropy

Plastic anisotropy is most pronounced and of greatest practical importance in rolled sheets, both with and without annealing treatments, and most experimental data relate to sheet samples in various deformation modes. A yield criterion based on a continuum mechanical approach for anisotropic materials exhibiting orthotropic symmetry (as do most sheet materials) was proposed by Hill [124]. In this treatment the tensile and shear yield stresses with respect to the symmetry axes are treated as parameters to be determined. The theory takes no account of the crystallographic nature of plastic flow, and has been criticized on this account [125]. It does, however, provide a simple means of understanding the behaviour of anisotropic materials in complex deformation modes. Hill demonstrated that the parameters could be
determined without a measurement of the through thickness tensile strength if the ratio of width to thickness strains (R) in tensile tests in the plane of the sheet were measured.

Since the strain ratio R is a comparatively easy parameter to measure it has been widely used to correlate the behaviour of materials in complex deformation modes with the behaviour in tensile tests. Lankford et al [126] showed that the drawability of a sheet, expressed in terms of the limiting ratio of blank size to punch diameter that could be successfully deep drawn, was correlated with $\bar{R}$, the mean value of R in the plane of the sheet. The heights of ears formed in deep drawn cups were shown by Bourne and Hill [127] to be related to the R values measured in the circumferential direction within the blanks.

Whiteley [128] showed that the correlation of $\bar{R}$ with drawability was consistent with Hill's yield criterion. Recent results have shown, however, that Hill's theory gives poor agreement with experimental results especially under complex stress conditions (e.g. [129,130]). Hosford and Backofen [131] suggested that a simpler and more theoretically sound correlation of drawability with texture could be made if $\beta$, the ratio of the strengths under the (approximately) plane strain strain conditions existing in the cup wall and flange respectively, were considered instead of $\bar{R}$. They showed that the limiting drawing ratio (LDR) should be given by

$$\ln (LDR) = \frac{\beta}{(1 + \eta)}$$

where $\eta$ is a friction parameter. $\beta$ is more difficult than $\bar{R}$ to measure experimentally, but Hosford and Backofen showed that it is more easily related to crystallographic texture. Wilson [114] has also indicated that relative strengths are of more direct interest than relative R values.
7.3.4 Correlation with Crystallographic Texture

The role of crystallographic texture in producing plastic anisotropy has been understood qualitatively for many years (see e.g. [1], Chapter 11). A quantitative method of relating $R$ with the distribution of slip directions was proposed by Burns and Heyer [132], and the method was used to correlate $R$ with the $\{111\}$ pole figures of low carbon steels [133]. Hosford and Backofen [131] showed that this method was based on an erroneous way of resolving strains. They suggested that a better method for predicting the behaviour of tensile specimens cut from a rolled sheet was to consider a fixed strain increment in the direction of the tensile axis, and to compute the work required to impose this increment as a function of the strain ratio. That value for which the work done was a minimum corresponded to the expected value, and the tensile strength could be obtained from the work done at that minimum value. The work done was determined by the Bishop and Hill analysis, with the contribution from each orientation present weighted according to the amount of material in that orientation. Hosford and Backofen demonstrated the method for several ideal orientations. There will in fact be shear strain components in tensile tests on specimens cut obliquely to the sheet symmetry axes, and these are not accounted for in this approach. The work of Bourne and Hill [127] indicates that these components will introduce errors of only minor importance.

Crystallographic considerations indicate that a high $\overline{R}$ is obtained both in fcc and bcc metals when there are $\{111\}$ and $\{110\}$ texture components in the plane of the sheet [134]. Held [135] has shown that a good correlation is obtained between $\overline{R}$ and the ($\{111\} / \{100\}$) intensity ratios determined from inverse pole figure measurements in low
carbon steels.

Svensson [136] used Taylor's [77] results for the yield strength in axisymmetric tension, along with the assumed ideal orientations \{311\}<112> plus \{110\}<112> in order to predict the yield stress anisotropy of cold rolled aluminium. The variation in R with direction in the sheet was predicted by applying the Hill yield criterion [124] to the results for the yield stress. Although Svensson admitted that his predictions were only a first approximation, he showed that the choice of ideal orientations to fit the pole figure data could make a significant difference to the predicted anisotropy.

A yield criterion for anisotropic materials has been developed by Crans [137] and used to predict the yield stress anisotropy and plastic strain tensor of cold rolled copper foils tested in tension. The criterion only takes account of the distribution of slip planes, and the anisotropy of the distribution of slip directions is not considered. This probably explains the poor agreement of the predictions with experimental results.

A simple model of polycrystalline deformation has been proposed by Nagashima et al. [138]. This assumes that slip will occur in any given crystal when the Schmid factor of any slip system exceeds 0.25, and that the amount of slip is proportional to the Schmid factor. This enabled them to calculate a parameter D (which is related to the strain ratio R) for a crystal in any given orientation. They computed the D values corresponding to various reflections in an inverse pole figure measured by the Harris method [12], and found the weighted mean (the weighting factor was the measured intensity of the particular reflection). Reasonable agreement was obtained with experimental results for cold rolled steel sheets. It was considered that the Taylor theory
would have been a better model of polycrystalline plasticity, but that the calculations were too complex.

Recently Bunge and Roberts [23] have used an analysis based on that described by Hosford and Backofen [131], but taking into account the complete crystallite orientation distribution function determined by the method of Bunge [45] from X-ray pole figures. They showed that good agreement was obtained with experimental data for stabilized steel sheet. Kallend and Davies [118,139] have used a similar analysis, using Roe’s method of determining the crystallite orientation distribution function [44], to predict plastic anisotropy in textured sheets of fcc metals. They also found satisfactory agreement with experiment. The method used is described in Chapter 8.
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CHAPTER 8

CORRELATION OF ANISOTROPY WITH TEXTURE - THEORETICAL

8.1 Introduction

The absence of suitable theories linking single crystal properties with the properties of aggregates, and the inability to describe quantitatively the texture of a polycrystalline aggregate, have both proved stumbling blocks to the correlation of anisotropic properties with crystallographic texture. For both elastic and plastic properties there are still no generally applicable exact theories linking the properties of single crystals and polycrystals. Easily evaluated upper and lower bound solutions to both of these problems have, however, been established. There is no justification, either experimental or theoretical, for considering either the upper bound or the lower bound solution for elastic properties as being more nearly correct. In the case of plastic properties the upper bound solution (that of Taylor [77] and Bishop and Hill [102,103]) is theoretically more rigorous than the lower bound solution (due to Sachs [107]), and is approached closely by experimental data [101,121,122].

The problem of obtaining a quantitative description of texture has found an effective solution in the analyses of Roe [44], Bunge [45], and Williams [46], along with the availability of suitable digital computers on which to perform the calculations. The correlation of texture with certain elastic and plastic properties of sheets of copper and copper-zinc alloys has been investigated, using the orientation distribution analysis of Roe. The method used is described in this chapter.
8.2 The General Problem

Consider any anisotropic property, $g$, of a single crystal, whose orientation dependence is given by

$$ g = g(\psi, \Theta, \phi) $$

where $\psi$, $\Theta$, and $\phi$ are the Euler angles relating the crystal axes with the reference frame in which the property is measured (see Figs. 1.1 and 3.1). Provided that $g$ is an additive property, that interaction between crystals is negligible or accounted for in the evaluation of $g$, and that no contribution is made by material in grain boundaries,

$$ \overline{g} = \frac{1}{N} \sum_{r=1}^{n} g(\psi_r, \Theta_r, \phi_r) F(\psi_r, \Theta_r, \phi_r) \quad (8.1) $$

where

$$ N = \sum_{r=1}^{n} F(\psi_r, \Theta_r, \phi_r) $$

and $\overline{g}$ is the mean value of $g$ over $N$ crystals in $n$ orientations, and $F(\psi_r, \Theta_r, \phi_r)$ is the number of crystals in the $r$th orientation considered. When $n$ and $N$ are very large (as in a typical polycrystalline metal sample) the summation may be replaced by integration over all orientations. Putting $\xi = \cos \Theta$, equation (8.1) becomes:

$$ g = \frac{1}{A} \int \int \int g(\psi, \xi, \phi) F(\psi, \xi, \phi) \, d\psi \, d\xi \, d\phi $$

where

$$ A = \int \int \int F(\psi, \xi, \phi) \, d\psi \, d\xi \, d\phi $$

and since

$$ w(\psi, \xi, \phi) = F(\psi, \xi, \phi) / A $$

where $w(\psi, \xi, \phi)$ is the crystallite orientation distribution function,
this becomes

\[ g(\psi, \xi, \phi) = \int g(\psi, \xi, \phi) w(\psi, \xi, \phi) d\psi d\xi d\phi \quad (8.2) \]

Pursey and Cox [22] and Sturcken and Croach [140], who have considered the similar problem for textures exhibiting axial symmetry, have shown that expressions such as equation (8.2) may be evaluated easily provided that both \( g(\psi, \xi, \phi) \) and \( w(\psi, \xi, \phi) \) may be expanded in a series of spherical harmonics. Here these expansions are:

\[ g(\psi, \xi, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} G_{l,m,n}(\xi) e^{-im\phi -in\psi} \quad (8.3a) \]

\[ w(\psi, \xi, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} W_{l,m,n}(\xi) e^{-im\phi -in\psi} \quad (8.3b) \]

where \( G_{l,m,n}, W_{l,m,n} \) are coefficients (see Chapter 3, section 3.2). Because of the orthogonality of these functions, equation (8.2) becomes:

\[ \bar{g} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} G_{l,m,n} W_{l,m,n} \]

If the reference axes with respect to which the property is measured are rotated by the Euler angles \( \alpha, \beta, \) and \( \gamma \) with respect to those in which the \( W_{l,m,n} \) have been evaluated, the new coefficients \( W'_{l,m,n} \) are related to the \( W_{l,m,n} \) by [44]:

\[ W'_{l,m,n} = \left( \frac{2}{2l+1} \right)^{1/2} \sum_{p=-l}^{l} W_{l,m,n}(\cos \beta) e^{ip\alpha -i\gamma} \]

For the particular case of the variation of properties in the plane of a rolled sheet, where the original reference axes were the rolling, transverse, and normal directions respectively, \( \beta = \gamma = 0, \) and \( \phi \) is the angle between the new \( x \) axis and the rolling direction. By substitution in equation (A3) of Roe [44]
\[ Z_{lpm}(i) = 0, \ m \neq n = \left(\frac{2l+1}{2}\right)^{\frac{1}{2}}, \ m = n \]

and consequently

\[ \bar{g}(\alpha) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} G_{lmn} W_{lmn} e^{-im\alpha} \]

When the \( G_{lmn} \) and \( W_{lmn} \) are all real, this reduces to

\[ \bar{g}(\alpha) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} G_{lmn} W_{lmn} \cos m\alpha \quad (8.4) \]

In order to evaluate equation (8.4) the coefficients \( W_{lmn} \) and \( G_{lmn} \) must be determined. The \( W_{lmn} \) may be obtained by spherical harmonic analysis of pole figure data (see Chapter 3), and the \( G_{lmn} \) can be determined from

\[ G_{lmn} = \frac{1}{4\pi^2} \int \int \int g(\Psi, \xi, \phi) Z_{lmn}(\xi) e^{im\Psi} e^{inh} d\Psi d\xi d\phi \quad (8.5) \]

The function \( g(\Psi, \xi, \phi) \) will remain invariant under the operation of crystallographic symmetry elements, and consequently there will be restrictions on the possible values of \( G_{lmn} \). There are further restrictions on \( G_{lmn} \) if the property under consideration exhibits symmetry in its reference frame (e.g. Young's modulus in a given direction in a crystal is unchanged by a rotation of the crystal about that direction). In practice it is necessary to truncate the series expansion in equation (8.3a) after a finite number of terms. The effect of this on equation (8.4) is not very great since usually both \( G_{lmn} \) and \( W_{lmn} \) are convergent, and their product will converge even more rapidly.
8.3 Elastic Anisotropy

The orientation dependence of elastic modulus in cubic crystals is governed by the function
\[ Y = l_1^2 + l_2^2 + l_3^2 \]
where \( l_i \) is the direction cosine relating the direction considered with the \( x_i \) axis. This function can be shown to depend only on zeroth and fourth order spherical harmonics [22], and consequently equation (8.3a) becomes

\[ Y(\psi, \xi, \phi) = \sum_{\ell=0}^{4} \sum_{m=1}^{l} \sum_{n=1}^{l} G_{\ell m n} Z_{\ell m n}(\xi) e^{i \ell \psi} e^{i m \phi} \]

The mean value of \( Y(\psi, \xi, \phi) \) over all the crystals in a textured sheet for a given direction in the sheet is given from equation (8.4).

\[ \overline{Y}(\alpha) = 4\pi \sum_{\ell=0}^{4} \sum_{m=1}^{l} \sum_{n=1}^{l} G_{\ell m n} \overline{W}_{\ell m n} \cos(m \alpha) \quad (8.6) \]

The Voigt [24] and Reuss [25] average moduli can be obtained by inserting the value of \( \alpha \) for the particular direction in the sheet considered into the expression for the particular modulus required [141]. The Reuss average Young's modulus is given by:

\[ E_R = \frac{1}{s_{11} - 2(s_{11} - s_{12} - 0.5 s_{44}) Y} \quad (8.7) \]

and the Voigt average Young's modulus by:

\[ E_V = \frac{(c_{11} + 2c_{12})(c_{11} - c_{12} - 3Y c)}{(c_{11} + c_{12} - Y c)} \quad (8.8) \]

where \( c = c_{11} - c_{12} - 2c_{44} \).
Equation (8.5) was used to determine the coefficients $G_{lmm}$ of the expansion of $\gamma(\psi, \zeta, \phi)$. The function was evaluated at 6 degree intervals in $\psi, \Theta$, and $\phi$, and the integration was performed numerically. The values of the independent coefficients are:

\[
\begin{align*}
G_{000} &= 0.283 \\
G_{400} &= -0.035 \\
G_{410} &= 0.037 \\
G_{440} &= -0.049
\end{align*}
\]  

This method of determining the anisotropy of Young's modulus is equivalent to, but slightly simpler than the method used by Bunge [116] who has evaluated the effective elastic constants ($\overline{c}_{ijkl}$ and $\overline{e}_{ijkl}$) of the sheet as an intermediate step. There are 9 independent elastic modulus tensor elements in a sheet with orthotropic symmetry and consequently 36 spherical harmonic coefficients must be determined rather than 4 as in equation (8.9). Bunge's method is slightly more flexible, however, since it is readily possible to determine the elastic behaviour of the sheet under complex loading conditions from the effective elastic constants of the sheet.

8.4 Plastic Anisotropy

8.4.1 Lower Bound Solution

The lower bound solution for the correlation of single crystal flow stress with that of a polycrystal is due to Sachs [107]. The individual crystals in the aggregate are assumed to be subject to a uniform stress, equal to the applied stress, and yield is presumed to be governed by the Schmid law [120].
For a tensile test on a specimen cut from a rolled sheet, the $x$, $y$, and $z$ axes are taken to be the specimen longitudinal direction, width direction, and normal direction respectively, and $g(\psi, \theta, \phi)$ of equation (8.1) becomes the tensile stress in the $x$ direction (relative to the critical resolved shear stress) necessary to produce yield on the most favourable slip system in a crystal with a given orientation. In this work, $g(\psi, \theta, \phi)$ was determined at 6 degree intervals in the angular coordinates, using the Schmid law, for fcc crystals assuming slip on $\{111\}<110>\text{ slip systems (}\{110\}<111>\text{ slip in bcc crystals would lead to the same result, see, for example, Groves and Kelly [142]). The coefficients } G_{nm} \text{ were determined from equation (8.5) by numerical integration for } l < 14, \text{ and the predicted variation of flow stress in the plane of the sheet is given by equation (8.4).}

8.4.2 Upper Bound Solution

An upper bound solution for the relation between polycrystal plastic behaviour and single crystal plastic behaviour was given by Taylor [77]. An equivalent, but simpler method was devised by Bishop and Hill [102,103]. These methods enable the work done in imposing a given plastic strain increment to be calculated, assuming that the resolved shear stress on at least five independent systems must reach, but not exceed, the critical shear stress for slip. The method of Bishop and Hill has been described frequently in the literature (e.g. [101, 102, 103, 110, 122, 131]) and only a brief description will be given here.

The amount of plastic work per unit volume done by a tensile or compressive stress $\sigma_{xx}$ in the $x$ direction is

$$dw = \sigma_{xx} \ d\varepsilon_{xx} \quad (8.10)$$
where $d\varepsilon_{xx}$ is the incremental strain in the $x$ direction. This may be equated with the work due to shear on the active slip systems

$$dw = \tau \sum_i d\gamma_i$$

(8.11)

where $\tau$ is the critical stress for slip, assumed to be the same for all systems, and $d\gamma_i$ is the incremental shear on the $i$th system. Equations (8.10) and (8.11) yield

$$M = \frac{\sigma_{xx}}{\tau} = \frac{\sum_i d\gamma_i}{d\varepsilon_{xx}} = \frac{dw}{\tau d\varepsilon_{xx}}$$

(8.12)

$M$ is a generalized Schmid factor (the Taylor factor) relating the applied stress for flow with the critical stress for slip. Equation (8.11) may be written

$$\tau = \frac{dw}{\sum_i d\gamma_i}$$

For slip to occur, the shear stress must be raised to, but not above, the critical value for slip. It may be seen that this is achieved by minimising the total shear $\sum_i d\gamma_i$ (Taylor's principle) or by maximizing the work $dw$ (Bishop and Hill's principle).

Bishop and Hill showed that only a limited number of stress states are capable of fulfilling the yield criterion, and that state which maximises the work done in the imposed strain is the active stress state. Stress states have been given which satisfy the yield criterion for $\{11\}<110>$ slip $[110]$, $\{11\}<112>$ slip and twinning $[143]$ and $\{123\}<111>$ slip $[144]$. In all of these cases it is possible to interchange the slip planes and directions without invalidating the
results. When the active state has been found, the Taylor factor $M$ may be determined from equation (8.12).

In order to apply the analysis to textured sheets Hosford and Backofen [131] have suggested that values of $M$ should be determined for a given strain increment $d\varepsilon_{xx}$ in the direction of loading, as a function of $r$, where

$$r = \frac{d\varepsilon_{yy}}{d\varepsilon_{yy} + d\varepsilon_{zz}} = \frac{R}{1 + R}$$

where $d\varepsilon_{yy}$, $d\varepsilon_{zz}$ are strains in the width and thickness directions respectively. The minimum value of $\bar{M}(r)$ corresponds to the expected behaviour, and the values of $\bar{M}(r)$ and $r$ at the minimum identify the relative strength $\sigma_{xy}/\sigma$, and the strain ratio $R$.

For the purposes of this investigation, equation (8.4) becomes

$$\bar{M}(r, \alpha) = \frac{4\pi^2}{3} \sum_{l=0}^{\infty} \sum_{m=0}^{l} \sum_{n=0}^{l} G_{lmn}^m \cos m \alpha$$

The values of $G_{lmn}^m (r)$ were determined for values of $r$ of 0, 0.1, 0.2, ... 1.0, for $l \leq 14$. Only $\{111\}<110>$ slip was considered.

The mean absolute values of $G_{lmn}^m (r)$ for various orders, $l$, are given in Table 8.1. from which it may be seen that the fourth order coefficients are, on average, an order of magnitude larger than those of any other order which gives rise to anisotropic behaviour (zero order coefficients give rise to orientation independent properties). The variation of the independent fourth order coefficients with $r$ is shown in Fig. 8.1.
Figure 8.1. Variation of the fourth order coefficients $G_{4,m}(r)$ of the expansion of the function describing flow stress anisotropy according to the Bishop and Hill theory, with contraction ratio $r$. 

**TABLE 8.1**

<table>
<thead>
<tr>
<th>ORDER</th>
<th>MEAN ABSOLUTE VALUE OF $G_{1mn}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>4.471</td>
</tr>
<tr>
<td>4</td>
<td>0.191</td>
</tr>
<tr>
<td>6</td>
<td>0.012</td>
</tr>
<tr>
<td>8</td>
<td>0.022</td>
</tr>
<tr>
<td>10</td>
<td>0.003</td>
</tr>
<tr>
<td>12</td>
<td>0.005</td>
</tr>
<tr>
<td>14</td>
<td>0.003</td>
</tr>
</tbody>
</table>
Although the Taylor/Bishop and Hill analysis is theoretically more rigorous than the Sachs analysis, it is necessary to consider the limitations of this method. The basic assumptions of the theory are that deformation is homogeneous, and that the hardening behaviour of all active slip systems is the same and depends only on the total amount of prior slip.

The observed shape changes of individual grains during polycrystalline deformation are frequently different from that of the polycrystal itself, and this may be expected to be a reasonable objection to the theory. These deviations appear to occur in such a way as to lower the total amount of work, leaving the predicted values as an upper bound. The assumption that work hardening depends only on the total amount of prior slip might be questioned in view of the different combinations of slip systems and dislocation interactions that would prevail in differently oriented grains. However, experimental results indicate that perturbations due to differential hardening are within the limits of accuracy of the experiments [121,122].

8.5 Summary

Satisfactory methods are available for the correlation of the elastic and plastic properties of single crystals with polycrystals. Methods are given whereby these analyses can be applied to materials exhibiting preferred orientation, described by the crystallite orientation distribution function. As has been stated by Bunge and co-workers [23,116], the correlation of properties with orientation is facilitated if the crystallite orientation distribution analysis is performed by spherical harmonic methods (e.g. [44,45]).
9.1 Introduction

In Chapter 8 methods were described whereby the effect of crystallographic texture on the elastic and plastic properties of a polycrystalline aggregate of crystals exhibiting cubic symmetry could be assessed. These methods have been used to predict the planar anisotropy of Young's modulus and flow stress in textured sheets of copper, Cu - 10 percent Zn (gilding metal) and Cu -30 percent Zn (brass). The predictions are compared with the experimentally determined anisotropy of these properties in order to determine the validity of the methods used.

9.2 Anisotropy of Young's Modulus

The planar anisotropy of Young's modulus in 90 percent cold rolled sheets of copper, gilding metal, and brass, was determined by the transverse resonant vibration method described in Chapter 2, section 2.5.1. The coefficients $W_{lm}$ of the crystallite orientation distribution function were determined for the three materials from X-ray pole figure data as described in Chapter 3, and the orientation distribution functions of these materials are illustrated in Figs. 5.17, 5.24, and 5.31.

The Voigt, Reuss, and Hill average Young's moduli were calculated as described in Chapter 8, section 8.3. The values of the single crystal elastic constants were obtained from Aleksandrov and Ryzhova [145]. The variation in the predicted moduli with direction in the rolling plane are given, together with the experimentally determined
Young's modulus, in Figs. 9.1, 9.2, and 9.3 for the copper, gilding metal, and brass respectively.

The experimentally determined values of Young's modulus are seen to lie parallel with the predicted values, between the Reuss and Hill averages, for all three materials. This indicates that the angular variation in Young's modulus is accounted for very well by the methods used, although the absolute values are not. This is in agreement with the findings of Bunge and co-workers [23,116,117].

Figure 9.4 shows the predicted variation of Young's modulus in the rolling plane for 95 percent cold rolled copper. The crystallite orientation distribution function for this material is shown in Fig. 5.18. Also shown are the experimentally determined values of Young's modulus in the rolling plane for 96 percent cold rolled copper as determined by Weerts[18], and for 96 percent cold rolled Cu - 1 percent Zn, determined by Alers and Liu [19]. Again, the predicted results are in reasonable agreement with experimental data.

9.3 Anisotropy of Flow Stress

The anisotropy of 0.2 percent proof stress in the rolling plane of 90 percent cold rolled copper, gilding metal, and brass was determined by tensile tests as described in Chapter 2, section 2.5.2. The predicted flow stress anisotropy was calculated using the Sachs and the Bishop and Hill averaging procedures (Chapter 8, section 8.4). These methods both predict the flow stress in terms of a critical shear stress for the material. A sensible value of this for the multiple slip processes in polycrystals was not known for any of the materials, so the predicted values have been normalized and presented as the ratio of the stress in a given direction to that in the rolling direction. These
Figure 9.1. Angular variation of Young's Modulus in the rolling plane of 90 percent cold rolled copper, together with the predicted variation according to the Voigt (V), Reuss (R), and Hill (H) averaging procedures.

Figure 9.2. Angular variation of Young's Modulus in the rolling plane of 90 percent cold rolled gilding metal, together with the predicted variation according to the Voigt (V), Reuss (R), and Hill (H) averaging procedures.
values, together with the similarly normalized experimental data, are given in Figs. 9.5, 9.6, and 9.7. In absolute terms it must be remembered that the mean ratio of the Sachs average to the Bishop and Hill average is 2.2:3.06, so the predicted flow stresses using these two methods are, in fact, widely separated.

In all of the materials tested the flow stress anisotropy predicted by the Bishop and Hill analysis is seen to agree satisfactorily with the experimentally determined data. Similar agreement was found by Bunge and Roberts [23] in an analysis, based on the equivalent minimum shear principle due to Taylor [77], of the flow stress anisotropy in stabilized steel sheet, and also by Kallend and Davies [139] in an analysis of the flow stress anisotropy of annealed sheets of copper and Cu-brass.

The predictions of the Sachs analysis, on the other hand, do not give a very good agreement with the experimental data. Kocks [101] has shown that on an absolute scale, the polycrystalline yield stress is far closer to the upper bound (Taylor/Bishop and Hill) solution than to the lower bound (Sachs) solution, and the present results would seem to confirm this. Kallend and Davies [139] found that the anisotropy predicted by the Sachs average was in fair agreement with the experimentally observed flow stress anisotropy in annealed sheets of copper and brass. Since the predictions of the Sachs and Bishop and Hill methods were very similar in those cases, this agreement was probably fortuitous.
Figure 9.3. Angular variation of Young's Modulus in the rolling plane of 90 percent cold rolled brass, together with the predicted variation according to the Voigt (V), Reuss (R), and Hill (H) averaging procedures.

Figure 9.4. Predicted angular variation of Young's Modulus in the rolling plane of 95 percent cold rolled copper, together with the experimental results of Weerts (full circles) and of Aleris and Liu (open squares).
Figure 9.5. Angular variation of 0.2 percent proof stress in the rolling plane for 90 percent cold rolled copper, together with the predicted variation using the Sachs (S) and the Bishop and Hill (B-H) averaging procedures.

Figure 9.6. Angular variation of 0.2 percent proof stress in the rolling plane for 90 percent cold rolled gilding metal, together with the predicted variation using the Sachs (S) and the Bishop and Hill (B-H) averaging procedures.
Figure 9.7. Angular variation of 0.2 percent proof stress in the rolling plane for 90 percent cold rolled brass, together with the predicted variation using the Sachs (S) and the Bishop and Hill (B-H) averaging procedures.
9.4 Discussion

9.4.1 Elastic Properties

The results of the present work, together with those of Bunge and co-workers [23, 116, 117] and of Kallend and Davies [118] show that the variation of Young's modulus in the rolling plane of a polycrystalline sheet can be correlated satisfactorily with the sheet texture. It is not possible, however, to predict the absolute value of Young's modulus, although the Hill average [26] is probably the best approximation. Bunge et al. [117] have considered the effect of crystallite shape on Young's modulus, and have shown that deviation from an equiaxed grain structure will lead to anisotropy in Young's modulus in addition to that due to crystallographic texture. Should the grains be elongated in the direction of measurement the assumptions of the Voigt analysis are more nearly fulfilled, leading to a higher Young's modulus value, and vice versa. In a cold rolled material this would have the effect of increasing Young's modulus values in the rolling direction compared with those in the transverse direction. There is some evidence for this in Figs. 9.1, 9.2, and 9.3, although such small effects are not significant within the accuracy of the analysis.

The agreement between the predicted elastic anisotropy for 95 percent cold rolled copper and the experimental results of Weerts [18] and Alers and Liu [18] is of interest, since Alers and Liu found that a reasonable agreement with these data was obtained if the texture was considered to be 100 percent \( <523 \). However, the orientation distribution function (Fig. 5.18) shows that this is a wholly inadequate description of the copper texture. This illustrates the point made by Bunge and Roberts [23] that Young's modulus anisotropy is insufficiently sensitive to texture variations to be unequivocal as a method of texture...
9.4.2 Plastic Properties

The observed orientation dependence of flow stress in cold rolled sheets of copper, gilding metal, and brass, is described poorly by the Sachs model of polycrystalline plasticity. The Sachs averaging procedure is not well founded theoretically \[101\] and experimental results have shown that it does not correspond to the observed behaviour of 'random' polycrystals in measurements of absolute flow stress \[108\]. The present results show that in addition it does not in general predict an angular variation in flow stress in textured sheets which is in accord with experimental data.

The Bishop and Hill model of polycrystalline plasticity predicts a flow stress variation in the plane of the sheet which is in reasonable agreement with experimental data. Similar agreement has been found in stabilized steel sheets by Bunge and Roberts \[23\] and in annealed sheets of copper and brass by Kallend and Davies \[139\].

It is unlikely that the accuracy of the analysis could be improved simply by increasing the number of terms in the series expansion in equation (8.3a) since, as is shown in Table 8.1, the series converges very rapidly. It is also doubtful whether the inclusion of other deformation modes in addition to \{11\}<110> glide would increase the accuracy in fcc metals, since additional assumptions would have to be made concerning the relative prominence of the different modes considered (the most likely additional deformation mode would be \{11\}<112> twinning). Applying the analysis to bcc metals involves the assumption that slip is restricted to \{11\}<111> systems. In fact slip is observed on \{11\}, \{12\}, and non crystallographic planes in bcc...
metals [146], although apparent slip on these planes may be due to frequent cross slip of screw dislocations from one \{110\} plane to another [147]. Bunge and Roberts [23] suggested that consideration of deformation modes in addition to \{110\}<111> could improve the accuracy of their predictions.

As described in Chapter 8, section 8.4.2, the contraction ratio, $r$, in a tensile test on a sheet specimen is given by the value of $r$ at the minimum of the function $\tilde{M}(r)$ [131]. Since this function is very flat near the minimum [23] the value of $r$, and consequently of the strain ratio $R$, is subject to quite large errors as a result of small errors in the evaluation of $\tilde{M}(r)$. However, the results of Bunge and Roberts [23] showed that the form of the curve relating the contraction ratio with angle from the rolling direction was in agreement with observed data in stabilized steel sheets, and Kallend and Davies [139] predicted $R$ values for cube textured copper sheet that agree reasonably well with the values measured by Sauer and Wassermann [148] in copper sheet with a similar texture.

9.4.3 Practical Applications

There is a growing interest in the control of anisotropy of mechanical properties in sheet metals, so that optimum performance is obtained either in subsequent forming operations or in service conditions. Control of crystallographic texture is one of the principal methods of improving mechanical behaviour in sheet metals (see e.g. [114]) but the evaluation of sheet textures in the light of the required properties is hindered in most cases by the complexity of the textures produced by typical production processes. The use of the crystallite orientation distribution function to correlate crystallographic texture with properties, as described in Chapter 8, could clearly be of
assistance in the evaluation of sheet textures for specific purposes. Equation (8.4) shows that no contribution to planar anisotropy is made by those coefficients \( W_{lmn} \) of the series expansion of the distribution function when \( m = 0 \), and no contribution to normal anisotropy is made by coefficients \( W_{lmn} \) when \( m \neq 0 \). The actual effect of any particular coefficient \( W_{lmn} \) is dependent on the sign and magnitude of the corresponding \( G_{lmn} \) (see equation 8.3). This will be illustrated by some examples.

Equations (8.6), (8.8), and (8.9) show that in a sheet of any cubic metal for which the elastic anisotropy constant \( A \) is greater than unity \( (A = \frac{2c_{44}}{c_{11} - c_{12}}) \) [149], this includes most cubic metals, exceptions being niobium, molybdenum, and vanadium) a high value of Young's modulus in the plane of the sheet will occur when \( W_{400} \) is negative, and vice versa. A positive \( W_{420} \) leads to high Young's modulus in the rolling direction, with a low value in the transverse direction, while a positive \( W_{440} \) leads to high values at 45 degrees to the rolling direction. In a steel sheet, for example, maximum sheet stiffness in the rolling direction would be given by a large negative \( W_{400} \), a large positive \( W_{420} \), and a large negative \( W_{440} \).

The evaluation of plastic properties is slightly more complex, since the \( G_{lmn} \) for \( l > 4 \) are not all zero as in the case of elastic properties. Table 8.1 shows, however, that the fourth order coefficients are an order of magnitude larger than those of higher orders, and as a result fourth order terms will dominate equation (8.13). Hosford and Backofen [131] showed that good drawability in sheets of cubic metals is obtained when a parameter \( \beta \) is large (see also Chapter 7, section 7.3.3). \( \beta \) is given by:
Hosford and Backofen also showed that $\beta$ is more closely related to the drawing process than the strain ratio $R$, since $R$ is only related to drawability through the Hill theory \[124\] whereas $\beta$ is related to drawability through consideration of the relative strengths of the cup wall and flange based on crystallographic criteria. Fig. 8.1 shows that a large negative $W_{400}$ will lead to a large $\beta$, and consequently to a high drawability, and vice versa, for the case of $\{111\}<110>$ or $\{110\}<111>$ slip. A positive $W_{420}$ leads to earing at $0$ and $180$ degrees from the rolling direction, and a positive $W_{440}$ leads to ears at $0$, $90$, and $180$ degrees. A good drawing quality material should have a large negative $W_{400}$. $W_{420}$ and $W_{440}$ should in general be as small as possible unless planar anisotropy is specifically desired as, for instance, in the case of anisotropic drawing operations (see \[114\]). In the latter case the ideal values for these coefficients could be determined for the particular operation envisaged, and the sheet texture optimized as far as possible by control of process variables.

Similar reasoning will apply in the case of texture hardening \[150\] in which the yield strength of the sheet under a typical loading condition (typically biaxial tension) is increased by control of texture. Balanced biaxial tension corresponds to the case $r = -1$, and by extrapolation from Fig. 8.1 it is expected that a negative $W_{400}$ would lead to the desired properties in fcc or bcc metals. The scope for texture hardening is greater in non-cubic metals because of their restricted deformation modes \[131\]. There does not yet seem to be any way of extending the Bishop and Hill analysis to hexagonal metals, and the best approach to this problem would probably be empirical, perhaps in a way similar to that used by Nagashima et al. \[136\] for bcc metals.

\[ \beta = \frac{M(r=0)}{M(r=1)} \]
CHAPTER 10

CONCLUSIONS AND SUGGESTIONS FOR FUTURE WORK

10.1 Introduction

A summary of the conclusions drawn from the results of this work on the applications of the crystallite orientation distribution function are presented in this chapter. Suggestions are made for future work which could improve the understanding of the development of textures and of the properties of textured sheet metals.

10.2 Conclusions

10.2.1 The Development of Rolling Textures in FCC Metals

The crystallite orientation distribution function provides an easily interpreted and unambiguous representation of sheet textures. The development of the cold rolling textures in copper, Cu - 10 percent Zn, and Cu - 30 percent Zn has been followed using the crystallite orientation distribution analysis due to Roe [44]. The texture of cold rolled copper is best described as a continuous range of orientations between \{110\}<112> and \{4 4 11\}<11 11 8>, and increasing deformation up to 95 percent reduction serves only to sharpen the texture. The copper alloys both exhibit an initial texture development similar to that of the copper, but at deformations greater than about 40 percent there is a depletion of orientations at the \{4 4 11\}<11 11 8> end of the range, and an increase in components near \{111\}<112>, \{552\}<115>, and \{110\}<001>, with considerable orientation spread.

A computer simulation of the texture development in fcc metals has been made, assuming multiple \{111\}<110> slip. The effects of
material and process variables on the behaviour of slip dislocations have been considered, as has the possibility of mechanical twinning. It is concluded that the changes in dislocation behaviour due to a decrease in stacking fault energy are not per se responsible for the observed differences between the pure metal and the alloy type textures, but that increased difficulty both of dislocation cross slip and of dislocation intersection promotes mechanical twinning and the formation of deformation bands which are responsible for the texture transition.

10.2.2 Properties of Textured Sheets of Cubic Metals

Methods of correlating the crystallographic texture with anisotropy of elastic and plastic properties in sheets of cubic metals are given. It is shown that the predicted anisotropy of Young's modulus and flow stress in textured sheets of copper, Cu - 10 percent Zn and Cu - 30 percent Zn are in reasonable agreement with experiment.

The practical importance of the control of crystallographic texture in sheet products is discussed, and methods are proposed for assessing the suitability of sheet textures for particular applications.

10.3 Future Work

10.3.1 Texture Development

As described in Chapter 4, many theories have been advanced to account for the texture development in fcc metals and alloys. In the copper - zinc alloys investigated in this work the onset of mechanical twinning produced large orientation changes which made it impossible to assess the direct effects of changes in dislocation cross slip behaviour and stacking fault frequency. The effects due to these could be investigated by an analysis of the development of the rolling texture in
materials with a higher stacking fault energy, such as nickel and aluminium, and also by a complete analysis of texture formation in ordered Cu$_3$Au, which has a low effective stacking fault energy but cannot deform by mechanical twinning [96]. Further information about fcc deformation mechanisms could be obtained by rolling sheets with pronounced initial textures and observing the reorientations produced using three dimensional methods (c.f. [81]).

Body centred cubic metals show much less variation in rolling textures than do fcc metals [2]. The development of rolling textures in, for example, low carbon steel could be followed using the orientation distribution function, and compared with predicted textures based on various deformation modes. In a preliminary investigation a simulation of the rolling texture arising from $\{110\}<111>$ slip has been made, following similar lines to that described in Chapter 6. Fig. 10.1 shows the predicted texture after 60 percent reduction, and Fig. 10.2 shows the texture of 60 percent cold rolled low carbon steel, determined by Goodwill [151]. There is reasonable agreement between the predicted texture and the experimentally determined texture for this material. The effect of slip on $\{112\}$ and $\{123\}$ planes, and of pencil glide, should be investigated, to see if the predicted textures arising from these deformation modes give a better fit with experimental data than does $\{110\}<111>$ slip alone.

10.3.2 Properties of Textured Materials

Further research activities in this field would best involve applications of the analytical methods described in Chapters 8 and 9 to technological problems. The inter-relations between sheet texture and behaviour during forming operations such as stretch forming and deep drawing could be studied, in order to identify the optimum values of
Figure 10.1. Predicted orientation distribution arising from multiple \{110\}<111> slip at 60 percent reduction. Constant $\phi$ sections.
Figure 10.2. Crystallite orientation distribution function for 60 percent cold rolled low carbon steel. Constant $\phi$ sections. Contours at intervals of 0.5.
material and process variables in the production of sheet metals. Hexagonal metals, such as titanium, could be studied in order to understand the nature and formation of the optimum textures for texture hardening, with the aim of extending the range of metals in which this form of hardening can be utilised.

Hoddinott and Davies [20] suggested that elastic modulus measurements could provide a rapid means of assessing quality during the production of deep drawing steels. Stickels and Mould [21] have demonstrated that an empirical relationship between Young's modulus anisotropy and $R$ values can be established. It should be possible to obtain an analytical relationship between these properties through equations (8.6), (8.7), (8.8), and (8.13). As a preliminary investigation the coefficients $W_{400}$ and $W_{440}$ of the orientation distribution function were obtained from the Young's modulus data of Stickels and Mould [21] using equations (8.6), (8.7), and (8.8). It was not possible to obtain an accurate estimate of $W_{400}$ in view of the uncertainty of the elastic modulus averaging procedure. Equation (8.13) was used to predict the $R$ values from these coefficients, the value of $W_{400}$ being allocated to make the predicted $\bar{R}$ equal to the measured $\bar{R}$. Table 10.1 shows the predicted $R$ values, along with the experimental results of Stickels and Mould. Agreement is seen to be good. Stickels and Mould have used the parameters $A_0^R$, $A_1^R$, and $A_2^R$ to characterize the behaviour, where

\[
A_0^R = 0.25[R(0) + 2R(45) + R(90)]
\]
\[
A_1^R = 0.5[R(0) - R(90)]
\]
\[
A_2^R = 0.25[R(0) - 2R(45) + R(90)]
\]

and have used the standard deviation between the predicted and measured values of these parameters as an indication of the goodness of fit of
## TABLE 10.1

Values of Strain Ratio (Experimental values after Stickels and Mould [21])

<table>
<thead>
<tr>
<th>STEEL IDENTITY</th>
<th>EXPERIMENTAL</th>
<th>PREDICTED</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>R(0)</td>
<td>R(45)</td>
</tr>
<tr>
<td>8</td>
<td>0.963</td>
<td>0.883</td>
</tr>
<tr>
<td>9</td>
<td>1.153</td>
<td>0.823</td>
</tr>
<tr>
<td>10</td>
<td>1.096</td>
<td>0.873</td>
</tr>
<tr>
<td>11</td>
<td>1.20</td>
<td>0.813</td>
</tr>
<tr>
<td>12</td>
<td>1.18</td>
<td>0.85</td>
</tr>
<tr>
<td>13</td>
<td>1.29</td>
<td>0.88</td>
</tr>
<tr>
<td>14</td>
<td>1.08</td>
<td>1.03</td>
</tr>
<tr>
<td>15</td>
<td>1.252</td>
<td>0.974</td>
</tr>
<tr>
<td>16</td>
<td>1.345</td>
<td>1.135</td>
</tr>
<tr>
<td>17</td>
<td>1.605</td>
<td>0.97</td>
</tr>
<tr>
<td>18</td>
<td>1.405</td>
<td>1.200</td>
</tr>
<tr>
<td>19</td>
<td>1.615</td>
<td>1.055</td>
</tr>
<tr>
<td>20</td>
<td>1.835</td>
<td>1.02</td>
</tr>
<tr>
<td>21</td>
<td>1.63</td>
<td>1.12</td>
</tr>
<tr>
<td>22</td>
<td>1.895</td>
<td>1.22</td>
</tr>
<tr>
<td>23</td>
<td>1.80</td>
<td>1.29</td>
</tr>
<tr>
<td>24</td>
<td>1.78</td>
<td>1.335</td>
</tr>
<tr>
<td>25</td>
<td>1.928</td>
<td>1.327</td>
</tr>
<tr>
<td>26</td>
<td>1.645</td>
<td>1.405</td>
</tr>
</tbody>
</table>

Note: only the values which are obtained from two or more specimens have been used.
their empirical relation. In this work $A_0^8$ has not been predicted, but has been set to the experimental value. $A_i^8$ and $A_i^6$, however, have been determined from the predicted $R$ values. The standard deviations between the predicted and measured $A_i^8$ and $A_i^6$ are given in Table 10.2. This shows that the analytical method described gives as good a fit with the experimental data as the empirical approach due to Stickels and Mould.

The uncertainty in $W_400$ could be eliminated for materials with an equiaxed grain structure by making a through thickness measurement of Young's modulus. This could be done, for example, with a longitudinal vibration method [152], and further work could be done to improve this method and assess its suitability as a rapid and simple means of quality control.
TABLE 10.2

Standard Deviations in $A_1^r$ and $A_2^r$

<table>
<thead>
<tr>
<th></th>
<th>Stickels and Mould (empirical)</th>
<th>Predicted from $W_{lmn}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1^r$</td>
<td>0.1123 (35 samples)</td>
<td>0.094 (26 samples)</td>
</tr>
<tr>
<td></td>
<td>0.0922 (32 samples)</td>
<td></td>
</tr>
<tr>
<td>$A_2^r$</td>
<td>0.0565 (35 samples)</td>
<td>0.074 (26 samples)</td>
</tr>
<tr>
<td></td>
<td>0.0564 (32 samples)</td>
<td></td>
</tr>
</tbody>
</table>
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APPENDIX 1

COMPUTER PROGRAM TO CALCULATE THE COEFFICIENTS $W_{\text{lmn}}$ OF THE CRYSTALLITE ORIENTATION DISTRIBUTION FUNCTION

This program computes the coefficients $W_{\text{lmn}}$ for values of $l$ up to and including 20 from pole figure data read in from input stream 1. The coordinates of the poles considered are read from input stream 5. The coefficients $Q_{\text{lmn}}$ are determined, as described in Chapter 3, section 3.3, by the instructions up to label 17. The remainder of the program determines the coefficients $W_{\text{lmn}}$, by solution of the simultaneous equations given in equation (3.10).

[PROGRAM TO ANALYSE POLE FIGURE DATA INTO SPHERICAL HARMONICS
AND DERIVE COEFFS. OF CRYSTALLITE DISTRIBUTION FUNCTION.
DI=POLE FIGURE DATA AT 5 DEGREE INTERVALS OF POLAR COORDS.
DS=POLAR COORDS OF CRYSTAL POLES BEING ANALYSED.
Q1=POLE FIGURE COEFFS
Q3=CRYSTAL DISTN. FN. COEFFS FOR PRINTER
Q4=DI FOR RE-INPUT]

[DETERMINE NORMALIZING FACTORS FOR SPHERICAL HARMONICS]

0: W[0]=1
FOR K=1:1:140;
W[K]=KW[K+1]
REPEAT
FOR L=0:1:10;
FOR M=0:1:10;
N=11L+M
*W[N]=SORT((4L+1)*W[L+L+M+M]/2W[L+L+M+M])
REPEAT
REPEAT
FOR R=0:1:399;
*Q1[R]=0.
REPEAT
1: N=100
D=0

[READ IN POLE FIGURE DATA]
2: FOR I=0:1:17
FOR J=0:1:17
R=18I+J
*I[124:D+R]=INPUT
IF /
REPEAT
REPEAT
2: D=D+1

[DETERMINE POLE FIG. COEFFS: Q1M) BY INTEGRATION]
3: D=1:1
FOR L=0:1:10
FOR M=0:1:10
N=11L+M
*ZS=100.
FOR S=0:1:1323;
Z=5 INTPT(8/18)
=9 IF: Z=S
=4: IF: *ZS=S
X=COS(RADIANS(Z))
=7.
C[1]=P
X=COS(RADIANS(Z+5))
=7.
C[2]=P
=9.
X=COS(RADIANS(Z+5))
SUBROUTINE TO GENERATE SPHERICAL HARMONIC PNS

5: T=(1-X)/2
A=2(N-L)
B=2(L+M)+1
C=2N+1
D=E=F=1
D=DAB*T/CD.
P=F+D
A=A+1
B=B+1
C=C+1
E=E+1
+6 IF Θ>Α.
+T2=1
++T=N=TT
FOR T=I:1:M
+T2=T2+T
REPEAT
+P=F*T2
RETURN

SUBROUTINE TO GENERATE INTEGRAL OF SPHERICAL HARMONICS

7: T=(1-X)/2.
*K=1
W[699]=1
FOR Θ=1:1:1+L+L+1
W[699+Θ]=W[599+Θ]*T.
REPEAT
+9 IF N=NS:
*Ν=Ν.
FOR Θ=0:1:1+L+L+1.
REPEAT
FOR Θ=M:1:1+M+M.
*K=K+1
REPEAT
A=2(N-L)
A=2(L+M+1)
C=M+M+1
FOR Θ=1:1:1+L+L+M-M.
A=A+1.
B=B+1.
C=C+1.
E=E+1.
REPEAT
FOR Θ=M:1:1+M+M.
FOR Θ=0:1:1+L+L+M-M.
REPEAT
REPEAT
8: P=0
FOR Q=H;1;L  
*P=Q+2N*(4Q+Q)/N*(Q+1)  
REPEAT  
RETURN  

9: *INT=(C[2]-C[11])*N[N]  
*UL=RADIANS(90*PRPT(S/18)+5)  
*LL=RADIANS(90*PRPT(S/18))  
-13 IF N=0  
B=(SIN(2M*UL)-SIN(2M*LL))/2M  

[SUM OVER ALL ELEMENTS OF POLE FIGURE]  
10: FOR K=0;1;D  
*Q1[130K+N]=*Q1[130K+N]+8*I[324K+S]B *INT/2H  
REPEAT  
*ZS=Z  
REPEAT  
REPEAT  

[NORMALIZE POLE FIGURES BY SETTING INTEGRAL TO 4 PI]  
11: FOR K=0;1;D  
OUTPUT 0  
C=(1/2H SQRT(2))/*Q1[130K]  
TEXT:REFLECTION:  
PRINT(K+1)2;0  
CRLF  
TEXT:MULTIPLY BY:  
PRINT(4HC)3  
TEXT:TO NORMALIZE X-RAY DATA:  
CRLF  

(DETERMINE TRUNCATION ERROR IN POLEFIGS,.)  
*Q=*P=0  
FOR I=0;1;I7  
Q=18;  
*K=SIN(RADIANS(2.5+5I))RADIANS(5)RADIANS(5)  
FOR J=0;1;I7  
*Q=*Q+8*I[324K+Q+J]*I[324K+Q+J]*K  
REPEAT  
REPEAT  
FOR L=0;1;L0  
FOR M=0;1;L  
N=INTEGER(I1L+MOD(N))  
*P=*P+*Q1[130K+N]*Q1[130K+N]  
REPEAT  
REPEAT  
G=(*Q-2H*P)/4H  
TEXT:TRUNCATION ERROR =:  
PRINT(4HC SIGN(G) SQRT(MOD(Q)))3  
CRLF  
TEXT:RMS INTENSITY =:  
PRINT(4HC SQRT(*Q/4H))3  
CRLF  
CRLF  
OUTPUT 1  
FOR L=0;1;10  
FOR M=0;1;L.
N=11L+M
*=Q1[130K+N]=C*Q1[130K+N]
PRINT(L)2;0
PRINT(M)2;0;4
PRINT(*Q1[130K+N])5
CRLF
REPEAT
12: REPEAT
  REPEAT
    +14
13: B=UL=LL;
    +10
14: TEXT1/1
    OUTPUT 1
    TEXT1/1
    OUTPUT 0

[ESTIMATE TRUNCATION ERROR IN FUNCTION]
FOR L=0;1;10;
  W[900+L]=0.
FOR M=1;L+1;
  N=12L+INTEGER(MOD(M)).
FOR K=1;L+D
REPEAT
REPEAT
REPEAT
*WAY=0.
G=0
FOR L=0;1;10;
  +15 IF L=1
  W[900+L]=LOG(W[900+L])
*WAY=WAY+W[900+L]/10.
15: REPEAT
  FOR L=0;1;10;
    +16 IF L=1
    B=B+(W[900+L]=*WAY)*(2L-10.8)
    C=C+(2L-10.8)*(2L-10.8)
16: REPEAT
  B=8/3
  A=EXP(*WAY=10.8B)
  FOR L=22;2;36
    G=G+(L*0.5)*A*EXP(BL)
  REPEAT
TEXT: TRUNCATION ERROR IN W (RANDOM = UNITY) =;
PRINT(SH H SQRT(G))3
CRLF
FOR R=0;1;1350
  W[R]=0.
REPEAT

[READ IN POLAR COORDINATES OF POLES: MEASURED]
READER 5
LIBRARY 23(33)
FOR L=0;L+D:
X[I] = COS(RADIANS(INPUT))
*T[I] = RADIANS(INPUT).

REPEAT

[NOW DETERMINE W COEFFICIENTS]

17: *SUM = 0
FOR T = 0: 1: D
*SUM = SUM + Q1[13*I] / (2*N[0]*SQRT(2))
REPEAT
W[0] = SUM / (D + 1)

18: L = 2
   = 2
FOR M = 0: 1: 2
   J = 12*L + 11*M
   *SUM = 0
   FOR T = 0: 1: D
     K = 11*I
     *SUM = SUM + Q1[13*I + 22*M]*D / (*P[K]*N[22] + 0.5976143)*P[K + 2]*4
     *N[24] = COS(4*T[I])
   REPEAT
   W[J] = SUM / (D + 1)
   W[J + 2] = 0.5976143*W
REPEAT

19: FOR M = 0: 1
   W[121 + 11*M] = 0
   REPEAT
   = 21

20: FOR T = 0: 1: D
   X = X[I]
   FOR M = 0: 21: L
     = 5
     *P[I + M] = *P
   REPEAT
   FOR T = 0: 1: L
     D = SQRT((4*L + 1)/2)/2
   RETURN

21: L = 3
   = 2
FOR M = 0: 1: 3
   *SUM = 0
   FOR T = 0: 1: D
     K = 11*I
     *N[35] = COS(4*T[I])
   REPEAT
   J = 12*L + 11*M
   W[J] = SUM / (D + 1)
   W[J + 2] = 1.8768287*W
REPEAT

22: L = 4
   = 2
FOR M = 0: 1: 4
   *SUM = 0

-125-
J = 121L + 11 N
FOR I = 0; I ≤ L; I++
K = 11 I
* N[48] 2 COS (8 * T[I]) + 0.37605672 * P[K+2] * N[46] 2 COS (4 * T[I])
REPEAT
W = W [J] = SUM / (I+1)
W [I+2] = 0.37605672 W
W [I+4] = 0.57295971 W
REPEAT

23; L= 5
> 20
FOR M = 0; M < 5
J = 121 L + 11 M
SUM = 0
FOR I = 0; I < 11 M
K = 11 I
* N[59] 2 COS (8 * T[I]) + 1.0076629 * N[57] * P[K+2] * N[52] 2 COS (4 * T[I])
REPEAT
W = SUM / (I+1)
W [J] = W
W [I+2] = -1.0076629 W
W [I+4] = -1.1993588 W
REPEAT

24; L= 6
> 33 IF D = 0;
> 20
FOR M = 0; M < 6
J = 121 L + 11 M
FOR I = 0; I < 11 M
K = 11 I
* 8.1491514 * P[K+4] * N[76] 2 COS (8 * T[I])
* N[72] 2 COS (12 * T[I]) + 1.4423922 * P[K] * N[70] 2 COS (4 * T[I])
Y[I] = Q1 (130 I + 66 + M)
REPEAT
> 25;
> 20
[SET UP LEAST SQUARES EQUATIONS]
25; FOR S = 0; S < 4
> C[S] = R[S] = 0;
REPEAT
> 26 IF D ≠ S;
FOR I = 0; I < S
REPEAT
> 27
26: \*C[1]=A[0]
\*C[2]=B[0]
\*R[1]=Y[0]
27: \textbf{LIBRARY 6} \{ \textbf{2:} \*C[1]:\*R[1] \}
\textbf{RETURN}
28: \textbf{W[J]=R[1]}
\textbf{W[J+2]=R[2]}
\textbf{W[J+4]=0.81491514*R[1]-1.4423922*R[2]}
\textbf{W[J+6]=0.44279661*R[1]+0.34631689*R[2]}
\textbf{REPEAT}
29: \textbf{L=7}
\textbf{-20-}
\textbf{FOR \textbf{M}=0:1:7}
\textbf{J=121L+11M}
\textbf{*SUM=0}
\textbf{FOR \textbf{I}=0:1:1D}
\textbf{K=117}
\textbf{*SUM=\textbf{SUM}+\textbf{Q1}} \{ \textbf{130I}+77\textbf{I}\} \textbf{D}/\textbf{1}\*\textbf{N}[77] *\textbf{P}[K]=e/95815825*N[83] \textbf{D}
\textbf{*P[K+6]} \textbf{2} \textbf{CO}\textbf{S}(\textbf{12}\*\textbf{T[I]})=0.7891065*\textbf{P}[K+4]*\textbf{N}[81] \textbf{2} \textbf{CO}\textbf{S}(\textbf{4}\*\textbf{T[I]}) \textbf{D}
\textbf{=0.73536134*P[K+2]*N[79] \textbf{2} \textbf{CO}\textbf{S}(\textbf{4}\*\textbf{T[I]})}
\textbf{REPEAT}
\textbf{W=H[7]=SUM/(D+1)}
\textbf{W[J+2]=0.73336134W}^\textbf{0}
\textbf{W[J+4]=0.7891065W}^\textbf{0}
\textbf{W[J+6]=0.95815825W}^\textbf{0}
\textbf{REPEAT}
30: \textbf{L=8}
\textbf{-20-}
\textbf{FOR \textbf{M}=0:1:8}
\textbf{J=121L+11M}
\textbf{*AH=*BM=*YM=0}
\textbf{FOR \textbf{I}=0:1:1D}
\textbf{K=117}
\textbf{+0.63115165*P[K+6]*N[94] \textbf{2} \textbf{CO}\textbf{S}(\textbf{12}\*\textbf{T[I]}) \textbf{D}}
\textbf{+0.44976475*P[K+4]*N[92] \textbf{2} \textbf{CO}\textbf{S}(\textbf{8}\*\textbf{T[I]}) \textbf{D}}
\textbf{*B[I]=2*N[99]*P[K+2] \textbf{CO}\textbf{S}(\textbf{4}\*\textbf{T[I]})+0.49142669*P[K+8]} \textbf{D}
\textbf{+0.51799902*P[K+4]*N[92] \textbf{2} \textbf{CO}\textbf{S}(\textbf{8}\*\textbf{T[I]}) \textbf{D}}
\textbf{*Y[I]=D*Q1[130I+88+M]}
\textbf{REPEAT}
\textbf{-25-}
\textbf{W[J]=R[1]}
\textbf{W[J+2]=R[2]}
\textbf{W[J+4]=0.44976475*R[1]+0.51799902*R[2]}
\textbf{W[J+8]=0.42227944*R[1]+0.49142669*R[2]}
\textbf{REPEAT}
31: \textbf{L=9}
\textbf{-20-}
\textbf{FOR \textbf{M}=0:1:9}
FOR \( i = 1 \) TO 10:
\[ J = 121 + i \cdot 10 \]
\[ *= \text{FOR} \quad \text{M} = 0 \quad \text{TO} \quad 1 \]
\[ *= \text{FOR} \quad \text{K} = 0 \quad \text{TO} \quad 11 \]
\[ *= \text{FOR} \quad \text{L} = 0 \quad \text{TO} \quad 19 \]
\[ *= \text{FOR} \quad \text{N} = 10 \quad \text{TO} \quad 11 \]
\[ *= \text{FOR} \quad \text{M} = 0 \quad \text{TO} \quad 1 \]
\[ *= \text{FOR} \quad \text{K} = 0 \quad \text{TO} \quad 2 \]
\[ *= \text{FOR} \quad \text{L} = 0 \quad \text{TO} \quad 1 \]
\[ *= \text{FOR} \quad \text{N} = 3 \quad \text{TO} \quad 8 \]
[PRINT OUT COEFFICIENTS]

33: OUTPUT 3
LAYOUT 3:169:8
+34:
OUTPUT 4:
LAYOUT 4:169:8
+34:
PRINTSYN(15)
CRLF
+ 35
34: FOR \( i = 0 \quad \text{TO} \quad 10 \)
FOR \( m = 0 \quad \text{TO} \quad 11 \)
FOR N=0;L:N
PRINT(L)2:0
PRINT(M)2:0:6
PRINT(N)2:0:6
PRINT(N[121L+11N+M])8:
REPEAT
REPEAT
REPEAT
RETURN

[ESTIMATE EXPERIMENTAL ERRORS]
35: FOR L=0;1;10:
   C[L]=0
   REPEAT
   FOR Q=0;1;D:
      X=X[Q]
      ETA=+T[Q]
   END
   FOR N=0;1;L:
      *A = 2H SQR(2/(4L + 1))
      FOR M=0;2;L:
         *S = 37 IF M = 0.
         *C = *C + 2W[121L + 11N + M]*P*N[11L + M] COS(2M*ETA)
      END
   END
36: FOR N=0;1;L:
      *C = *C + W[121L + 11N]*P*N[11L]
   END
37: OUTPUT 0.
   CRLF
   CRLF
   TEXT: EXPERIMENTAL ERRORS IN Q COEFFS.
   CRLF
   D=B=0.
   FOR L=0;1;10:
      C[L]=C[L]/(2L+1)(D+1)
      B=B+(C[L]/6M)(2L+1)(2L+1)
      D=D+(C[L]/2)(2L+1)
      PRINT(L)2:0
      PRINT(SQR(C[L]))4.
   CRLF

-129-
REPEAT
CRLF
TEXT: AVERAGE ERROR IN POLEFIGS = 1
PRINT (4H SQRT(D))4
CRLF
TEXT: TOTAL ERROR IN W = 1
PRINT (6H SQRT(B))4
PAGE
STOP
START: 0
APPENDIX 2

COMPUTER PROGRAM TO CALCULATE AND PLOT THE
CRYSTALLITE ORIENTATION DISTRIBUTION FUNCTION

This program calculates the crystallite orientation distribution function at each of 2560 points on a three dimensional grid in $\psi$, $\theta$, and $\phi$, using equation (3.9). The generating formula for the generalized spherical harmonic functions is that given by Roe [44]. The function is normalized so that unity corresponds to a random orientation density, and the values are printed out. A suitable set of contour values is chosen, and the function is plotted in constant $\phi$ sections.
(PROGRAM TO PLOT W FUNCTION IN CONSTANT PHI SECTIONS)
OUTPUT ON 01 PRINTER, 06, 7 PLOTTER)

[READ IN COEFFICIENTS]
@; L=INPUT+1 IF: /
@; M=INPUT
@; N=INPUT
@; W[121L+11M+N] = INPUT
+; 0

[PRELIMINARY CALCULATIONS]
@; F[0]=1.
@; FOR K=1:1:40:
@; F[K]=F[K-1]*K:
@; REPEAT
@; READER 5
@; *STAR=INPUT
@; LIBRARY 16 (12:0:15)
@; *XS = 0

[RUN THROUGH ARRAY OF POINTS IN EULER SPACE]
@; FOR *TH = 0:6:190
@; X = COS(RADIANS(*TH))
@; FOR *PS = 0:6:190
@; Y = RADIANS (*PS)
@; FOR *PH=STAR:*PHS
@; Z = RADIANS (*PH)
@; R=INTEGER(256*PHS/16+16*TH/6+0S/6)

[DETERMINING COEFTS. OF SPHERICAL HARMONICS]
@; T = 0
@; W = 0
@; @; 3 IF X = *XS
@; @; T = (1 - X)/2
@; @; TI = T * T
@; @; T[0] = 1.
@; @; T[@; = 1.
@; @; FOR K = 1:1:20
@; @; T[K] = T[K-1]*T.
@; @; TI[K] = TI[K-1]*TI.
@; REPEAT

[SUBROUTINE TO GENERATE SPHERICAL HARMONICS]
@; FOR @; L = 0:1:10:
@; LL=121, L
@; L=2, L
@; FOR @; M = 0:1: L
@; M=2, M
@; FOR @; N = -M:1: M
@; N=2, N
@; P = LL + 11,M + INTEGER(MOD(@; N))
@; Q = LL + 11 INTEGER(MOD(@; N)) + M
@; 4 IF MOD(W[P]) > .00015
@; 4 IF MOD(W[@;]) > .00015
@; 10
4: 7 IF X = *XS
   I = M + N
   J = M + N
   G = *N*T[I]*T[J]
   A = M = L
   B = L + M + 1
   C = M = N + 1
   D = M = P = 1

5: D = DAB*T/CR
   F = P + D
   A = A + 1
   B = B + 1
   C = C + 1
   E = E + 1
   6 IF A >= 0
   5

6: *FG[T] = FG
   [FIND SUM OF THE SERIES, TAKING ADVANTAGE OF SYMMETRY]
7: 8 IF M = MOD(N)
   W = W + 2*FG[T]*W[P]*COS(MY + NZ) + W[Q]*COS(NY + NZ)
   10

8: 9 IF M = 0
   W = W + 2*FG[T]*W[P]*COS(MY + NZ)
   10

9: W = W + *FG[T]*W[P]

10: T = T + 1
    REPEAT
    REPEAT
    REPEAT
    *W[R] = 80H7
    15 IF *W[R] >= UPL
11: *X3=X
    REPEAT
    REPEAT
    REPEAT

   [DETERMINE RANGE OF FUNCTION, AND SET SUITABLE CONTOUR INTERVAL]
   *C = INTPT({UPL/6})
   19 IF *C = 0.
12: TEXT: UPPER LIMIT : ;
    PRINT({UPL}212
    CRLF
    TEXT: INTERVALS BETWEEN CONTOURS : ;
    PRINT({C}212
    CRLF

   [PRINT OUT VALUES OF FUNCTION AT GRID POINTS]
   OUTPUT 1.
   FOR L=0:1:4
   TEXT: VALUES OF W AT PHI= ;
   PRINT({10L}210
   CRLF

-133-
CRLF
CRLF
FOR T=9:1:15:
FOR J=0:1:15:
PRINT(*W[256]+16M+N])2;2;1.
REPEAT
CRLF
CRLF
REPEAT
PAGE
REPEAT.

[SELECT PLOTTER]
OUTPUT = 6

[LIBRARY ROUTINES FOR PLOTTING AND CONTOURING]
13: LIBRARY 16, (259+50+5)
   LIBRARY 26(0;0;0;3)
   LIBRARY 16(200;0;4)
   FOR M=9:256,1025:
   LIBRARY 16 (0;400;4)
   LIBRARY 24 (16;16;16;*W[M];C[0];20;20;90;0)
   = 16+
   REPEAT
   LIBRARY 16(0;600;2)

14: OUTPUT = 7
   LIBRARY 16 (0;0;7)
   LIBRARY 26(0;0;9;3)
   LIBRARY 16(19;0;15)
   LIBRARY 16(59;59;5)
   FOR M=9:256,1025:
   LIBRARY 16(0;500;4)
   LIBRARY 24 (16;16;16;*W[M];C[0];30;30;90;0)
   = 16+
   REPEAT
   LIBRARY 16(0;600;2)

15:*UPL=*W[R];
   =11

16:LIBRARY 23(1)
   FOR A = *C1*C1*UPL;
   = 17 IF A=1
   LIBRARY 23 (A)
17: REPEAT
   RETURN
18: LIBRARY 16 (5;10;1)
   LIBRARY 16 (19;5;1)
   = 17
19: *UP=INTEGER(*UPL)
   = UP[20;21;22;23]
   = 23
20: [DUMMY]
21:*C=9.1
   = 12
22:*C=9.25
   = 12
23:*C=9.5
   = 12
START 9
This program is an example of the programs used to calculate the anisotropy of properties from the crystallite orientation distribution function. The calculation is based on equations (8.6), (8.7), and (8.8). The coefficients $W_{i\alpha}$ are read in from input stream 2, the coefficients $G_{i\alpha}$ from input stream 4, and the single crystal elastic moduli from input stream 5. Young's modulus is calculated for various directions in the rolling plane, and the results are printed out.
PROGRAM TO CALCULATE YOUNG'S MODULUS IN THE PLANE OF THE SHEET ACCORDING TO THE VOIGT, REUSS, AND VRH AVERAGES
D2 = W COFFS OF MATERIAL DISTRIBUTION, FUNCT.
D4 = COFFS OF EXPANSION OF ELASTIC PROPS
D5 = SINGLE CRYSTAL CONSTANTS OF MATERIAL

[READ IN W1MN FOR MATERIAL]
0!L=INPUT + 1 IF /
M=INPUT
N=INPUT
W[12]L+11M+N#INPUT
= 6

[READ IN ELASTIC MODULUS TENSOR ELEMENTS FOR MATERIAL]
1: J=0
READER 5
*C11=INPUT
*C12=INPUT
*C44=INPUT
*C2=C11=*C12-2*C44
*S11=*C11*(C11+C12)-2*C12*C12) (*C11=C12)
*S11=(*C11+C12-C12+C12)*S
*S12=(*C12+C12-C12*C11)*S
*S44=1/C44

[READ IN INDEPENDENT G1MN FOR ELASTIC ANISOTROPY]
READER 4
FOR L=0;1;2
P=0

2: FOR M=0;1;L;
K=0

3: FOR N=0;2;P;
X=INPUT
X=INPUT
X=INPUT
A[K]=INPUT
K=K+1;
REPEAT
L{5;6;7}

4: J=J+7;
REPEAT
REPEAT
L 8

[DETERMINE DEPENDENT G1MN]
5:*TF[J]=A[0]
I=1
I=4
6:*TF[J]=0
I=1
I=4
7:*TF[J]=A[0]
*TF[J+1]=A[0]+0.5976143
I=2
I=4
[*TH IS ANGLE FROM ROLLING DIRECTION]

8: FOR *TH=0 TO 180 DEGREES
   *RTH=RADIANS(*TH)
   TEXT: VALUE OF YOUNG'S MODULUS AT
   PRINT (*TH) 2.0
   TEXT: DEGREES FROM R.D.
   *SUM=0
   J=0

[FIND SUM OF PRODUCTS OF COEFFICIENTS FOR GIVEN DIRECTION]

FOR L=0 TO 15:
   L=L+L
   FOR M=0 TO 15:
   FOR N=0 TO 15:
      M=M+M
      *W1=W[(12*L+11*N+12)*COS(M*RTH)
      10 IF *M=0.
      11 IF *N=0.
      *SUM=SUM+4*N1*TF(J)
      9
      J=J+1.
      REPEAT
      REPEAT
      REPEAT
      13
      10: 12: IF *N=0.
      *SUM=SUM+2*N1*TF(J)
      9
      11: SUM=SUM+2*N1*TF(J)
      9
      12: SUM=SUM+N1*TF(J)
      9
      13: *GAMMA=SUM/N(0) SOFT(2)

[SUBSTITUTE MEAN VALUE OF GAMMA IN EXPRESSION FOR YOUNG'S MODULUS]
   *ERBUSS=R/(S11-S12-0.5*S44)*GAMMA
   *EVIOGT=(S11+C12)/(S11+C12)+3*GAMMA*CAV)/(C11+C12)*GAMMA*CAV

[PRINT OUT RESULTS]
CRLF
CRLF
TEXT: REUSS
PRINT (*ERBUSS) 4
CRLF
TEXT: VOIGT
PRINT (*EVIOGT) 4
CRLF
TEXT: HILL
PRINT ((*ERBUSS+*EVIOGT)/2) 4
CRLF
CRLF
REPEAT
STOP
START 0
APPENDIX 4

COMPUTER PROGRAM TO SIMULATE ROLLING TEXTURE DEVELOPMENT

The program given in this appendix is that which simulates the development of rolling texture when multiple \{11\}<110> slip, and mechanical twinning on \{11\}<112>, are permissible deformation modes. The operation of the program is as described in Chapter 6, section 6.4.
PROGRAM A29 E9 D9 *SA(3) *SB(3) *SC(3) *.
*A(1)*SH(9)*APT(9)*SD(3) *TH(150°) *RAND(3)

[CRYSTAL ROTATIONS UNDER IMPOSED ROLLING STRAIN]

[INITIALISE COMPUTATION]

*PI=H:
READER 5
.TWIN=INPUT
OUTPUT 1.
LAYOUT 1:60;6.
H=0
*RAND=0.4
*CHANGE=*RAND:
R=0

[IMPOSED STRAIN TENSOR FOLLOWS]

E[1]=0.05
E[9]=--0.05

[GENERATE UNIFORM INITIAL CRYSTAL DISTRIBUTION]

FOR *THS=3;9;90
*THS=*THS.
Y=RADIANS(*THS)
*INT=12/SQRT(SIN(Y))
FOR *PSS=1;INT;99.
*PS=*PSS
Y=RADIANS(*PSS)
FOR *PHS=1;INT;99.
*PH=*PHS
*QS=100
*SSS=0
*STRAIN=0
Z=RADIANS(*PHS)
*CA=COS(Y)
*SA=SIN(Y)
*CB=COS(Y)
*SB=SIN(Y)
*CC=COS(Z)
*SC=SIN(Z)

[SET UP TRANSFORMATION MATRIX FOR CRYSTAL]

*A[1]=CB*CA*CC--SA*SC
*A[8]=--SB*SA
1;*STRAIN=*STRAIN+0.05
*SSS=SSS=1

[DETERMINE STRAIN TENSOR FOR CRYSTAL]

FOR i=1;1;3
FOR j=1;1;3

-139-
\*SS=0
FOR P=1:1:3
FOR L=1:1:3
\*SS=\*SS+A[3L+P-3]*A[3J+L-3]*E[3P+L-3]
REPEAT
REPEAT
D[3I+J-3]=\*SS
REPEAT
REPEAT

[NOW RUN THROUGH B-H STRESS STATES AND DETERMINE MAX WORK STATE]
A=B=G=H=P=1
A=1
B=1
\* 6\*
B=1
\* 6\*
A=1
\* 6\*

2: P=1
\* 6\*
G=1
\* 6\*
H=1
\* 6\*

3: A=G=0,5:
B=1
\* 6\*
A=0,5:
G=0,5
B=1
\* 6\*
A=1:
B=F=G=0,5
\* 6\*
A=1:
B=0,5:
P=0,5
\* 6\*
A=B=G=0,5
\* 6\*
A=0,5:
H=0,5
\* 6\*

-140-
A = F = H = 0.5
→ 6 ←
A = H = 0.5
F = 0.5
→ 6 ←
A = F = 0.5
H = 0.5
→ 6 ←
A = 0.5
F = H = 0.5
→ 6 ←
A[16] = D
B = 0.5
G = H = 0.5
→ 6 ←
A[17] = D
B = G = 0.5
H = 0.5
→ 6 ←
A[18] = D
B = H = 0.5
G = 0.5
→ 6 ←
A[19] = D
B = G = 0.5
H = 0.5
→ 6 ←
A = 0.5
B = F = 0.5
→ 6 ←
A[21] = D
A = F = 0.5
B = G = 0.5
→ 6 ←
A[22] = D
A = G = 0.5
B = F = 0.5
→ 6 ←
A[23] = D
A = F = G = 0.5
B = 0.5
→ 6 ←
F = G = 0.5
H = 0.5
→ 6 ←
F = H = 0.5
G = 0.5
→ 6 ←
A[26] = D
F = 0.5
G = H = 0.5
\begin{verbatim}
6:
  A[27]=D
  F=G=H=0.5
  A[28]=D
  A = B*G = H

  A = B = G = H = 0
  RETURN

7:
  FOR i=1; i<28;
    8 IF D>MOD(A[i])
    D = MOD(A[i])
    *SIGN = SIGN(A[i])
    Q = I

8: REPEAT
   J = 9
   LIBRARY 2(*CHANGE)
   9 IF Q6*CHANCE*TSTRAIN=F3
   9 IF Q6*S3S=Q
   9 IF *TWIN=Q
   9

  [TEST WHETHER TWINNING LIKELY]

9:
  A = D[D][5] = D[9]
  B = D[D][9] = D[1]
  C = D[D][1] = D[5]
  F = D[D][6]
  G = D[D][7] = D[H][2]
  T = 3
  FOR i=1; i<12:
    19 IF *T>A[i]
    T = A[i]

10: REPEAT
   Q7
   LIBRARY 2(*CHANGE)

   [TWINNING PROBABILITY DETERMINED FROM TWINNING PARAMETER]
   19 IF Q7 = CHANCE*TSTRAIN = Q7 = D = SQRT(3)*/T
   LIBRARY 2(*CHANGE)
   Q7 = TWIN

   [CRYSTAL ROTATION ON TWINNING]
\end{verbatim}
FOR I=1:1:12:
A[I]=0
REPEAT
A[I,T]=1
=161:
→ 16 IF *CHANCE>0.5:
OUTPUT 0
TEXT: 'TWIN'.
OUTPUT 1
11: A=BC=2/3
→ 15
12: A=C=2/3; B=A
→ 15
13: A=B=2/3; C=A
→ 15
14: B=C=2/3; A=B
= 162:
, QS=100
A=B=C=0
16: *STRAIN=*STRAIN+0.11:
M=0
→ 17 IF 0.511=*STRAIN>0.025:
→ 17 IF *STRAIN=0.511+0.135:
→ 159:
17: M=500
→ 18 IF 0.916=*STRAIN>0.025:
→ 18 IF *STRAIN=0.916+0.135:
→ 159:
18: II=1699
→ 1 IF 1.61=*STRAIN>0.025:
→ 159:
→ 157:

[NOW CHOOSE SHEARS WITHIN PERMITTED LIMITS IN OPERATIVE STRESS: STAT]
FOR K=1:1:3
*S[A[K]]=*S[B[K]]=*S[C[K]]=*S[D[K]]=0
REPEAT
K=0
Q=Q=1
→ Q[26;28;36;44;50;56;62;69;76;83;90;97;104;]
105;108;111;112;115;118;121;124;127;130;133;136;141;146;154]

[STRESS STATE 1]:
J=J+1:
→ 152:

-143-
*V1=S.
  21 IF *V1*SIGN>*V3*SIGN
  *V1=*V3
21; *V2=D[5]=2D[7]
  *V3=*W2
  22 IF *V3*SIGN>*V2*SIGN
  *V2=*V3
22; *SA[1]=*V2+{*V1>*V2}*RAND
  *V1=0.
  23 IF *V1*SIGN>*V3*SIGN
  *V1=*V3
  *V3=*W2=*SA[1]
  24 IF *V3*SIGN>*V2*SIGN
  *V2=*V3
24: 152*
  *SB[1]=*V2+{*V1>*V2}*RAND
  29 IF =0.00001>*SB[1]*SIGN
  *V1=0.
  25 IF *V3*SIGN>*V1*SIGN
  *V1=*V3
25; *V2=D[1]+2D[6]
  152*
  26 IF *V2*SIGN>*V3*SIGN
  *V2=*V3
26; *SA[2]=*V2+{*V1>*V2}*RAND
  29 IF *SA[2]*SIGN=0.00001
  156

[STATE 2]
  J=J+1.
  152*
  *V1=0.
  29 IF *V1*SIGN>*V3*SIGN
  *V1=*V3
  30 IF *V3*SIGN>*V2*SIGN
  *V2=*V3
30; *SB[2]=*V2+{*V1>*V2}*RAND
  29 IF =0>*SB[2]*SIGN
  152*
  *V1=0.
  *V3=*SB[2]=*W1

-144-
31: IF \( V3 \cdot \text{SIGN} > V1 \cdot \text{SIGN} \)
\( V1 = V3 \)
\( = 32 \) IF \( V2 \cdot \text{SIGN} > V3 \cdot \text{SIGN} \)
\( V3 = V[3] \)
32: IF \( SB[3] = V2 + (V1 \cdot V2) \cdot \text{RAND} \)
\( = 28 \) IF \( SB[3] \cdot \text{SIGN} > 0 \cdot 000001 \)
\( V3 = V[3] \)
\( V1 = 0 \)
\( = 33 \) IF \( V1 \cdot \text{SIGN} > V3 \cdot \text{SIGN} \)
\( V1 = V3 \)
\( = 34 \) IF \( V3 \cdot \text{SIGN} > V2 \cdot \text{SIGN} \)
\( V2 = V3 \)
\( 34: SC[2] = V2 + (V1 \cdot V2) \cdot \text{RAND} \)
\( = 28 \) IF \( SB[2] \cdot \text{SIGN} = 0 \cdot 000001 \cdot SC[2] \cdot \text{SIGN} \)
\( = 36 \) IF \( J = 4 \)
\( = 37 \) IF \( V3 \cdot \text{SIGN} > V1 \cdot \text{SIGN} \)
\( V1 = V3 \)
\( V3 = V[2] \)
\( = 38 \) IF \( V2 \cdot \text{SIGN} > V3 \cdot \text{SIGN} \)
\( V2 = V3 \)
\( 38: SA[1] = V2 + (V1 \cdot V2) \cdot \text{RAND} \)
\( = 39 \) IF \( SA[1] \cdot \text{SIGN} = 0 \cdot 000001 \cdot V[0] \)
\( = 39 \) IF \( V1 \cdot \text{SIGN} > V3 \cdot \text{SIGN} \)
\( V1 = V3 \)
\( = 40 \) IF \( V3 \cdot \text{SIGN} > V2 \cdot \text{SIGN} \)
\( V2 = V3 \)
\( 40: SD[3] = V2 + (V1 \cdot V2) \cdot \text{RAND} \)
\( = 41 \) IF \( V3 \cdot \text{SIGN} > V1 \cdot \text{SIGN} \)
\( V1 = V3 \)

-145-
   $W_2 = V_3$
   $W_1 = 0$

42: $W_3 = 0$
   $W_2 = 0$
   $W_4 = W_5 = 0$

   $W_1 = 0$

44: $W_1 = 0$
   $W_4 = W_5 = 0$

45: $W_2 = 0$
   $W_4 = W_5 = 0$

   $V_2 = V_4 * V_3 * V_2 * (V_1 + V_3) * RAND$
   $W_2 = V_2$

47: $W_2 = V_1 + W_1 + W_2$

48: $W_3 = 0$
   $W_4 = W_5 = 0$

   $V_2 = V_1 + SB[2] + W_2$
   $W_3 = V_1$
   $SB[3] = V_2 + (V_3 * V_2 * RAND)$
   $W_3 = W_2$

   $W_3 = W_3$

51: $W_3 = 0$

-146-
52: IF \( *W3*SIGN > *W2*SIGN \)
\( *W2 = *W3 \)
53: IF \( *V1*SIGN > (D[5] + 2D[7]) *SIGN \)
54: IT \( *V2 = *V1 + *W1 + *W2 \)
55: IF \( *SA[1] = *V2 + (*V3 + *V2) \) *RAND \)
56: IF \( *W1 + *SA[1] = 0,00001 > 0 \)
\( *V2 = *V1 + *SA[1] + *W2 \)
57: IF \( *W3 = *W1 \)
\( *SD[3] = *V2 + (*V3 + *V2) \) *RAND \)
58: IF \( *W2 = *W3 \)
59: IF \( *SD[3] = *W3 \)
\( *V1 + *W2 \)
61: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
62: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
63: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
64: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
65: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
66: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
67: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
68: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
69: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
70: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
71: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
72: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
73: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
74: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
75: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
76: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
77: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
78: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
79: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
80: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
81: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
82: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
83: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
84: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
85: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
86: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
87: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
88: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
89: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
90: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
91: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
92: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
93: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
94: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
95: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
96: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
97: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
98: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
99: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
100: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
101: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
102: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
103: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
104: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
105: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
106: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
107: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
108: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
109: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
110: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
111: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
112: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
113: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
114: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
115: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
116: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
117: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
118: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
119: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
120: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
121: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
122: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
123: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
124: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
125: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
126: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
127: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
128: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
129: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
130: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
131: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
132: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
133: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
134: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
135: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
136: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
137: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
138: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
139: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
140: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
141: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
142: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
143: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
144: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
145: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
146: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
147: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
148: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
149: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
150: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
151: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
152: IF \( *V2 = *V1 + *SA[1] \) *RAND \)
\*V1=0,
\*V3=*W2

> 70 \ IF \ \*V1\*SIGN>*V3\*SIGN.
\*V1=*V3

70;\ \*V2=*D[5]-2D[7].
\*V3=*W1=*W3

> 71 \ IF \ \*V3\*SIGN>*V2\*SIGN.
\*V2=*V3

71;\ \*SB[3]=*V2+{*V1-*V2}\*RAND.
> 152;
\*V1=0.
\*V3=*W1=*W2

> 72 \ IF \ \*V1\*SIGN>*V3\*SIGN.
\*V1=*V3

72;\ \*V2=*D[5]=2D[7].
\*V3=*W3

> 73 \ IF \ \*V3\*SIGN>*V2\*SIGN.
\*V2=*V3

73;\ \*SA[1]=*V2+{*V1-*V2}\*RAND.
\*V1=0.

> 74 \ IF \ \*V3\*SIGN>*V1\*SIGN.
\*V1=*V3


> 75 \ IF \ \*V2\*SIGN>*V3\*SIGN.
\*V2=*V3

75;\ \*SA[2]=*V2+{*V1-*V2}\*RAND
> 69 \ IF \ 0.6666661>*SB[3]\*SIGN.

> 156

[STATE 9]
76;\ \*155; \ IF \ J=4.
J=J+1;
> 152;
\*V1=0.
\*V3=*W1=*W2

> 77 \ IF \ \*V1\*SIGN>*V3\*SIGN.
\*V1=*V3

\*V3=*W3;

> 78 \ IF \ \*V3\*SIGN>*V2\*SIGN.
\*V2=*V3

78;\ \*SA[2]=*V2+{*V1-*V2}\*RAND.
> 152;
\*V1=0.
\*V3=*W2

> 79 \ IF \ \*V1\*SIGN>*V3\*SIGN.
\*V1=*V3
\*V2=\*V3

89i: = 152-
\*SA(1)=\*V2+(\*V1=\*V2)*RAN
\*SD(2)=D[1]+2D[6]=SB(2)
*156.

[STATE 11]
90i: = 155 IF. J=4.
J=J+1.
*152-
\*W2=D[1]+2D[6]
\*W3=2D[7]+2D[5]
\*V1=0.
\*V3=\*W1+\*W2
*91 IF \*V1=SIGN>>V3=SIGN
\*V1=V3
*V3=\*W3
*92 IF \*V3=SIGN>>V2=SIGN
\*V2=V3
92: \*SA(1)=\*V2+(\*V1=\*V2)*RAN
*152-
\*V1=0.
\*V3=\*W1+\*W2
*93 IF \*V1=SIGN>>V3=SIGN
\*V1=V3
*V3=\*W2
*94 IF \*V3=SIGN>>V2=SIGN
\*V2=V3
94: \*SC(2)=\*V2+(\*V1=\*V2)*RAN
*90 IF \*SA(1)=SIGN
*V1=0.
*95 IF \*V3=SIGN>>V1=SIGN
\*V1=V3
*96 IF \*V2=SIGN>>V3=SIGN
\*V2=V3
96: = 152-
\*SA(3)=\*V2+(\*V1=\*V2)*RAN
*90 IF \*SA(3)=SIGN=0; 00001>*V1=SIGN
*156.

[STATE 12]
97i: = 155 IF. J=4.
J=J+1
  => 152:
    *V2=*D[1]+2D[7]-2D[2].
    *V3=*D[1]-2D[6].
    *V1=0.
    *V3=*V2
  => 98 IF *V1*SIGN>*V3*SIGN
      *V1=*V3

    *V3=*V1.*W1.*W3
  => 99 IF *V3*SIGN>*V2*SIGN.
      *V2=*V3

99:*X[1]=*V2+(*V1-*V2)*RAND.
    => 152:
      *V1=0.
      *V3=*W1.*W2.
    => 100 IF *V1*SIGN>*V3*SIGN.
      *V1=*V3

    *V3=*W3.
  => 101 IF *V3*SIGN>*V2*SIGN.
      *V2=*V3

101:*SA[2]=*V2+(*V1-*V2)*RAND.
    => 97 IF *SA[2]=SIGN.
      *V1=0.
    => 102 IF *V3*SIGN>*V1*SIGN.
      *V1=*V3

  => 103 IF *V2*SIGN>*V3*SIGN.
      *V2=*V3

103:*SA[3]=*V2+(*V1-*V2)*RAND.
    => 97 IF *SA[3]=SIGN=0.
    => 104 IF *V3*SIGN>*V1*SIGN.
      *V1=*V3

104: [DUMMY -STATE 13 NOT OPERATIVE ]
    => 179

    *V1=0.
    *V3=2D[6]-2D[7]+2D[2].
  => 106 IF *V1*SIGN>*V3*SIGN.
      *V1=*V3

    *V3=*D[5]-2D[7].
  => 107 IF *V3*SIGN>*V2*SIGN.
      *V2=*V3

J = J + 1
  = 152.
  /* J */
  *SA[1] = *V2 + (*V1 = *V2) *RAN.
  *V1 = 0.
  *V1 = *V3.
  *V2 = *V3.
  J = J + 1.
  = 152.
  /* J */
  *SC[1] = *V2 + (*V1 = *V2) *RAN.
  *V1 = 0.
  = 156.

111; (DUMMY -- STATE 16 NOT ACTIVATED)
  = 179.

[STATE 17]
  *V1 = *V3.
  *V1 = *V3.
  *V2 = *V3.
  114; = 155 IF, J = 2.
  J = J + 1.
  = 152.
  /* J */
  *SA[2] = *V2 + (*V1 = *V2) *RAN.
  = 156.

[STATE 18]
  = 153.
116: IF *V3*SIGN>*V1*SIGN.

117: IF *V2*SIGN>*V3*SIGN.

118: IF J=2:

J=J+1.

119: IF *V1*SIGN>*V3*SIGN.

120: IF *V3*SIGN>*V2*SIGN.


122: IF *V1*SIGN>*V3*SIGN.

123: IF *V3*SIGN>*V2*SIGN.

124: IF J=2:

J=J+1.

STATE 19


119: IF *V1*SIGN>*V3*SIGN.

120: IF *V3*SIGN>*V2*SIGN.

STATE 20


122: IF *V1*SIGN>*V3*SIGN.

123: IF *V3*SIGN>*V2*SIGN.

124: IF J=2:

J=J+1.

-154-
[STATE 21]
124; *S[3]=D{5}+2D{6}
*SD{3}=D{1}+2D{6}
*V1=0.
*V3=2D{6}+2D{7}+2D{2}
→ 125: IF *V3*SIGN>*V1*SIGN.
*V1=*V3
125; *V2=D{1}+D{5}+2D{2}
*V3=D{1}+D{5}+2D{6}-2D{7}
→ 126: IF *V2*SIGN>*V3*SIGN.
*V2=*V3
126; = 155: IF J=2:
J=J+1;
→ 152:
*SA{1}=*V2+(*V1=*V2)*RAND
→ 126: IF *SA{1}*SIGN=0.00001>*V1*SIGN.
*SA{2}==D{1}+D{5}+2D{2}+*SA{1}
*SD{2}=2D{6}+2D{7}+2D{2}+*SA{1}
*SD{1}=D{1}+D{5}+2D{6}-2D{7}==SA{1}
→ 156.

[STATE 22]
127; *SA{3}=D{1}+2D{6}
*SB{3}=D{5}+2D{7}
*V1=0.
*V3=2D{6}+2D{7}+2D{2}
→ 128: IF *V3*SIGN>*V1*SIGN.
*V1=*V3
128; *V2=D{1}+D{5}+2D{2}
*V3=D{1}+D{5}+2D{6}-2D{7}
→ 129: IF *V2*SIGN>*V3*SIGN.
*V2=*V3
129; = 155: IF J=2:
J=J+1;
→ 152:
*SA{1}=*V2+(*V1=*V2)*RAND
→ 129: IF *SA{1}*SIGN=0.00001>*V1*SIGN.
*SB{2}==D{1}+D{5}+2D{2}+*SA{1}
*SD{1}=D{1}+D{5}+2D{6}+2D{7}==SA{1}
*SD{2}=2D{6}+2D{7}+2D{2}==SA{1}
→ 156.

[STATE 23]
130; *SA{3}=D{5}+2D{7}
*SB{3}=D{1}+2D{6}
*V1=0.
*V3=2D{6}+2D{7}+2D{2}
→ 131: IF *V1*SIGN>*V3*SIGN.
*V1=*V3
131; *V2=D{1}+D{5}+2D{2}
*V3=D{1}+D{5}+2D{6}+2D{7}
→ 132: IF *V3*SIGN>*V1*SIGN.
*V2=*V3
132; = 155: IF J=2:
J=J+1;
→ 152:
*SA{2}=*V2+(*V1=*V2)*RAND.
132: IF *V1*SIGN=0,000001>*SA[2]>*SIGN
→ 156.

[STATE 24]
*V1=0.
→ 134. IF *V3*SIGN>*V1*SIGN.
*V1=*V3
→ 135. IF *V2*SIGN>*V3*SIGN.
*V2=*V3
135: 155 IF J=2:
J=J+1
→ 152:
*SB[1]=*V2+(*V1=*V2)*RAND
→ 135. IF *SB[1]*SIGN=0,000001>*V1*SIGN
→ 156.

[STATE 25]
→ 137. IF *V1*SIGN>*V3*SIGN.
*V1=*V3
→ 138. IF *V1*SIGN>*V3*SIGN.
*V1=*V3
→ 139. IF *V3*SIGN>*V2*SIGN.
*V2=*V3
139: 149 IF 0>*V2*SIGN:
*V2=0;
140:
140: 152:
*SA[1]=*V2+(*V1=*V2)*RAND
→ 155. IF *V1*SIGN=0,000001>*SA[1]*SIGN
→ 153. IF *SA[1]*SIGN=0,000001>*V2*SIGN
→ 156.

[STATE 26]
→ 142. IF *V1*SIGN>*V3*SIGN.
*V1=*V3
142: 143 IF *V1*SIGN>0:
*V1=0.

143: *V2=D[5]+2D[7];
> 144. IF *V3*SIGN>*V2*SIGN:
*V2=*V3
144: *V3=-2D[6]-2D[7]+2D[2];
> 145. IF *V3*SIGN>*V2*SIGN:
*V2=*V3
145: = 152:
*SA[1]=*V2+(*V1-*V2)*RAND
= 155. IF *SA[1]*SIGN>0.00001>*V2*SIGN
= 155. IF *V1*SIGN=0.00001>*SA[1]*SIGN.
> 156.

[STATE 27]
146: *V1=D[1]+2D[7]-2D[2];
> 147. IF *V3*SIGN>*V1*SIGN:
*V1=*V3
147: = 148. IF 0>*V1*SIGN:
*V1=0.
148: *V2=D[1]+2D[6];
*V3=D[1]+D[5]-2D[2];
> 149. IF *V2*SIGN>*V3*SIGN:
*V2=*V3
149: *V3=2D[6]+2D[7]-2D[2];
> 150. IF *V2*SIGN>*V3*SIGN:
*V2=*V3
150: = 152:
*SA[2]=*V2+(*V1-*V2)*RAND
= 155. IF *V2*SIGN<0.00001>*SA[2]*SIGN
= 155. IF *SA[2]*SIGN=0.00001>*V1*SIGN.
> 156.

151: = 179
[STRESS STATE 28 NOT ACTIVATED IN REGION CONSIDERED]

[GENERATE RANDOM NUMBER WITH LIBRARY ROUTINE 2]
152: = 153. IF *QS=Q
LIBRARY 2 (*CHANCE)
*RAND=*RAND[K]=INTPT(*CHANCE+0.499)
> 154.
153: *RAND=*RAND[K]
154: K=K+1
RETURN

[ERROR EXIT]
155: OUTPUT 0

-157-
Q=Q+1
TEXT: FAILURE TO OBSERVE BOUNDARY CONDITIONS:
STRESS STATE:
PRINT(Q*SIGN)2:0:
CRLF
TEXT: ORIENTATION:
PRINT(*THS)3:1
PRINT(*PSI)3:1
PRINT(*PHS)3:1
CRLF
CRLF
* 172:

[TEST WHETHER TOTAL REDUCTION IS 40, 60, OR 80%]

156: 160:
*QS=3
M=0
* 156: IF 0.025>MOD(*STRAIN=0.511)
M=500:
* 159: IF 0.025>MOD(*STRAIN=0.916)
M=1000:
* 159: IF *STRAIN>1.61
157: 158 IF M=1160
* 1
158: 172
159: 163:
+ 170:
M=M+100
* 157:

[ROTATION DETERMINED BY CURL OF DISPLACEMENT]

160: *DPS1=(*2*SA1)+*SA2)+*SA3)+*SB1)+*SB2)+*SB3)+*SC1)+*SC2)
+*SC3)+*SD1)+*SD2)+*SD3)0.25
*DPS2=(*2*SA1)+*2*SA2)+*SB1)+*SB2)+*SB3)+*SC1)+*SC2)
+*SC3)+*SD1)+*2*SD2)+*SD3)0.25
*DPS3=(*2*SA1)+*SA2)+*SB1)+*SB2)+*SB3)+*SC1)+*SC2)
+*SC3)+*SD1)+*SD2)+*SD3)0.25

161: *DPS=SQRT(*DPS1+*DPS2+*DPS3)
*CDP=COS(*DPS)
*SDP=SIN(*DPS)
*CRT=ARCCOS(*CDP)
*SRH=SIN(*CRT)
*V1=V2+*CDP
*V3=DSI+*DPS
LIBRARY 1(V3;V1;*RPH)
*SRPH=SIN(*RPH)
*CRPH=COS(*RPH)
*CRT2=CRTH*CRT
*SRTH=SRTH*SRTH
*CRPH2=CRPH*CRPH
*SRPH2=SRPH*SRPH

[DETERMINE REORIENTATION MATRIX]

*SH[1]=*CRT2*CRPH2*CDPH+*SRPH2*CDPH+*SRTH2*CRPH2
*SH[4]=*SRTH2*CRT2*CDPH*SRPH(1-*CDPH)=*SDPS+*CRT
*SH[7]=*SRTH(*SDPS+*SRPH+*CRPH+*CDPH+*CRTH+*CRPH)
*SH[2]=*CRT2*SDPS+*SRTH2*SRPH+*CRPH(1-*CDPH)
NOW DETERMINE NEW ORIENTATION MATRIX

[LOCATE ALL CRYSTALS WITHIN REGION OF EULER SPACE CONSIDERED]

[STORE FINAL COORDINATES]
R=R+1;

[PLOT RESULTS IN CONSTANT PHI SECTIONS]  
[PLOTTING LIBRARY ROUTINES FOLLOW]

*PLOT=6
FOR *M=0;500;1000:
OUTPUT *PLOT
LIBRARY 16(0;0;PLOT)
LIBRARY 16(10;0;15)
LIBRARY 26(0;0;9;3)
LIBRARY 16(50;0;15)
*PH=90:
->173
*PH=90:
->174:
FOR *PH=10;10;180:
->173
REPEAT
*PLOT=*PLOT+1:
REPEAT
->177
173;X=0;Y=500;N=4
->178
X=0;Y=0;N=2:
->178
X=300;Y=0;N=1:
->178
X=0;Y=300:
->178
X=0;Y=0:
->178
X=0;Y=300:
->178
174;FOR I=M;1;N+R
*AB=INTPT(*TH[I]/10000)/10 -*PH
->176 IF MOD(*AB)>5
X=(1000/3) FRPT(INTPT(*TH[I]/100)/100)
Y=(1000/3) FRPT(*TH[I]/100)
N=2
->178
->178
->175 IF *AB>0
N=3;X=3;Y=0:
->178
X=6;N=1
->178
->178
175;N=3;X=0;Y=3:
->178
Y=6;N=1
->178
176;REPEAT
RETURN:
177;STOP
178;LIBRARY 16(X;Y;N)
RETURN
179;->163
*CA=SOS(*PS)
*SA=SIN(*PS)
*CB=SOS(*TH)
*SB=SIN(*TH)
*CC=SOS(*PH)
*SC=SIN(*PH)
*A[1]=*CB*CA*CC-*SA*SC
*A[8]=*SB*SA
*STRAIN=*STRAIN-0,05:
-> 1

{ERROR EXIT IF TOO MANY CRYSTALS GENERATED FOR
ALLOCATED STORE}.
180:OUTPUT 0
TEXT:OVERFLOW PLOT SPACE:
PRINT(*TH)3;2:
PRINT(*PS)3;2:
PRINT(*PH)3;2:
CRLF
CRLF
= 172:
START:0.