

Thermal behaviour of diiron arsenide under non-oxidising conditions[†]

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Supporting Information

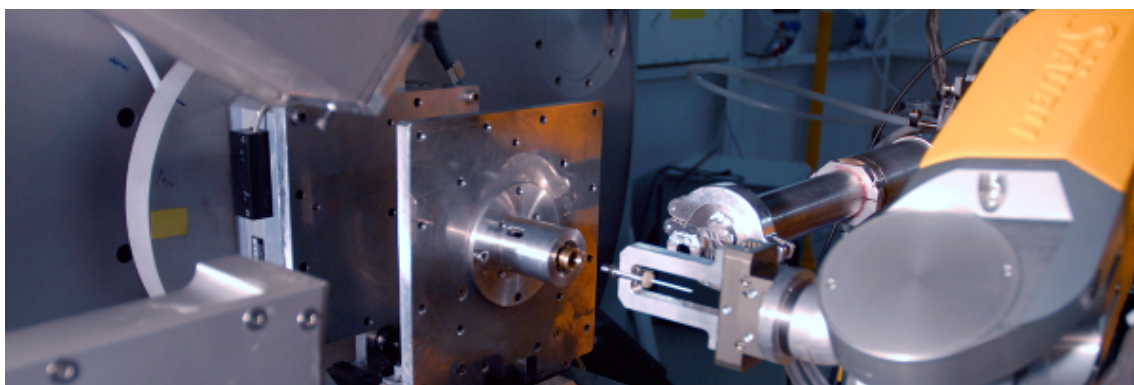


Figure S1: A picture of the powder diffraction experimental setup showing the solid-state silicon microstrip detector MYTHEN II (Microstrip sYstem for Time- rEsolved experimeNts) on the left

[†]Thermal behaviour of iron arsenides under non-oxidising conditions

Table S1: The starting crystallographic data

Phase	Chemical formula	Space group	ICSD coll. code	Reference
Iron arsenide (2/1)	Fe ₂ As	$P4/nmm$	415628	1
Iron arsenide (1/1)	FeAs	$Pna2_1$	15009	2
α -Fe	Fe	$Im - 3m$	53802	1
α -As	As	$R3m$	16516	3
Magnetite	Fe ₃ O ₄	$Fd - 3m$	82455	4
Wuestite	FeO	$Fm - 3m$	82233	5

Table S2: Cell parameters data for Fe₂As, FeAs, and Fe

Phase	Cell parameters, Å			Comments	Reference
	a	b	c		
Fe ₂ As	3.634	-	5.985	-	6
	3.627	-	5.985	-	7
	3.627	-	5.981	-	8
	3.63	-	5.98	-	9
	3.632	-	5.981	-	10
	3.634	-	5.985	-	11
FeAs	5.4420	3.3727	6.0278	at 20 °C	2
	5.437	3.370	6.023	-*	12
	5.439	3.373	6.028	-	13
	5.4401	3.3727	6.0259	-	14
	5.440	3.370	6.030	-	11
	5.432	3.372	6.023	-	8
	5.44	3.41	6.03	at 310 °C	8
	5.44	3.43	6.08	at 452 °C	8
	5.45	3.45	6.07	at 618 °C	8
	5.47	3.47	6.10	at 748 °C	8
	5.48	3.49	6.12	at 890 °C	8

* Neutron Diffraction.

Table S3: Dependence of cell parameters and volume of Fe₂As, FeAs from temperature

T, °C	a (Å)	b(Å)	c(Å)	V(Å)
Fe ₂ As				
50	3.6413	3.6413	5.9951	79.4903
100	3.6465	3.6465	6.0008	79.7925
150	3.6503	3.6503	6.0075	80.0487
200	3.6544	3.6544	6.0146	80.3238
250	3.6589	3.6589	6.0220	80.6199
300	3.6635	3.6635	6.0300	80.9302
350	3.6678	3.6678	6.0382	81.2309
400	3.6713	3.6713	6.0466	81.4964
450	3.6745	3.6745	6.0549	81.7523
500	3.6776	3.6776	6.0631	82.0032
550	3.6807	3.6807	6.0711	82.2509
600	3.6839	3.6839	6.0791	82.4979
650	3.6870	3.6870	6.0868	82.7421
700	3.6899	3.6899	6.0946	82.9813
750	3.6930	3.6930	6.1024	83.2263
800	3.6972	3.6972	6.1111	83.5320
850	3.7022	3.7022	6.1200	83.8807
FeAs				
200	5.4622	3.4097	6.0505	112.6877
250	5.4578	3.4191	6.0538	112.9686
300	5.4518	3.4260	6.0574	113.1382
350	5.4486	3.4329	6.0614	113.3739
400	5.4488	3.4405	6.0670	113.7346
450	5.4509	3.4482	6.0737	114.1603
500	5.4538	3.4557	6.0813	114.6131
550	5.4575	3.4637	6.0897	115.1150
600	5.4616	3.4718	6.0990	115.6462
650	5.4658	3.4800	6.1088	116.1957
700	5.4700	3.4888	6.1194	116.7820
750	5.4743	3.4982	6.1311	117.4110
FeAs(HT)				
800	3.9188	3.9188	5.3702	82.4691
850	3.9453	3.9453	5.3918	83.9242

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