The Nature of the Bonds in the Iron Silicide FeSi and Related Crystals*

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The iron silicide FeSi has been reinvestigated by X-ray photography of single crystals, and the reported structure for the substance has been verified. The space group is T^4-$P2_1 3$, with

$$a_0 = 4 \cdot 489 \pm 0 \cdot 005 \text{ A.}$$

Four iron atoms and four silicon atoms are in positions $(x, x, x; \ x + \tfrac{1}{2}, \tfrac{1}{2} - x, \bar{x}; \ \text{\textit{y}})$, with

$$x_{\text{Fe}} = 0 \cdot 1370 \pm 0 \cdot 0020 \quad \text{and} \quad x_{\text{Si}} = 0 \cdot 842 \pm 0 \cdot 004.$$

A detailed discussion of the structure and the values of the interatomic distances has been given, by application of the resonating-valence-bond theory, and it has been shown that the interatomic distances are compatible with those found for elementary iron and elementary silicon.

Introduction

The structure of the iron silicide FeSi was first investigated by Phragmén (1923), who found it to be based upon the space group T^4-$P2_1 3$, with a unit cell containing four iron atoms in the positions $(x, x, x; \ x + \tfrac{1}{2}, \tfrac{1}{2} - x, \bar{x}; \ \text{\textit{y}})$ and four silicon atoms in a similar set. The edge of the cubic unit cell (a_0) was given as 4·48 A., and it is evident from Phragmén's drawing of the structure that x_{Fe} and x_{Si} were taken as approximately $\tfrac{1}{8}$ and $\tfrac{5}{6}$. Wever & Moeller (1930) later studied this structure by use of powder photography and reported the values $x_{\text{Fe}} = 0 \cdot 1340 \pm 0 \cdot 0020$, $x_{\text{Si}} = 0 \cdot 8445 \pm 0 \cdot 0020$, and $a_0 = 4 \cdot 467$ A. (It is mentioned in the *Strukturbericht*, **2**, p. 241, however, that the authors have stated in a personal communication that an error was made in their determination of the parameters.) Another powder photographic study of this substance was made by Borén (1933), who reported $x'_{\text{Fe}} = 0 \cdot 139 \pm 0 \cdot 001$, $x_{\text{Si}} = 0 \cdot 845 \pm 0 \cdot 001$, and $a_0 = 4 \cdot 478$ A.

The structure found for FeSi and other silicides (CrSi, MnSi, CoSi, NiSi) (Borén, 1933) is interesting as an example of co-ordination number 7. Each iron atom is surrounded by seven silicon atoms, and each silicon atom by seven iron atoms, at the distances 2·28 A. (one ligand), 2·35 A. (3), and 2·50 A. (3) (calculated with the parameter values of Borén; those of Wever & Moeller lead to values agreeing with these to within 0·03 A.). Each iron atom also has six iron neighbors at 2·75 A. We became interested in the structure in connection with our efforts to develop a rational theory of metals and intermetallic compounds (Pauling, 1938, 1947), and attempted to find an explanation of the choice by these substances of this unusual structure, in preference to the sodium chloride, nickel arsenide, or cesium chloride structure, and also an explanation of the

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* Contribution no. 1172 from the Gates and Crellin Laboratories.

unusually small interatomic distances shown by the crystal. These small distances make themselves evident when an effort is made to calculate the valences of the iron and silicon atoms from the bond distances, with use of the recently proposed relation between bond distance and valence (Pauling, 1947):

$$R_n = R_1 - 0 \cdot 300 \log n. \tag{1}$$

The bond numbers obtained from the reported interatomic distances lead, when summed, to the valences 6·98 for iron and 6·93 for silicon, in obvious disagreement with those usually accepted, 5·78 and 4·00, respectively.

The seriousness of the apparent anomaly in valence and the incompleteness of the published details of the only single-crystal investigation of the structure that has been reported (Phragmén, 1923) caused us to consider the possibility of an error in the structure determination, and led us to verify the structure and to redetermine the parameters by single-crystal X-ray methods.

Experimental methods and results

A preparation which consisted of silicide crystals embedded in a silicon-rich α-iron matrix was made by slowly cooling a mixture of reagent-grade iron and silicon containing 25 (wt.) % of silicon from the molten state, under 40 mm. of hydrogen. A residue of silicide crystal fragments and silica was obtained by the decomposition of the sample with hot aqua regia. A single-crystal fragment with longest dimension less than 0·1 mm. was selected, and its individuality as a single crystal was demonstrated by the preparation of heavily exposed symmetrical Laue photographs. The Laue point group was found to be T_h-$2/m\bar{3}$. The value of a_0 was found to be $4 \cdot 489 \pm 0 \cdot 005$ A. from equatorial measurements of 15° oscillation photographs; no re-

flections requiring a larger cell were observed on the Laue or oscillation photographs.* The lattice is primitive, restricting the space group to

$$T^1{-}P23, \quad T^4{-}P2_13, \quad T_h^1{-}Pm3, \quad T_h^2{-}Pn3,$$

or $\quad T_h^6{-}Pa3$ (*Internationale Tabellen*...).

$T_h^2{-}Pn3$ is eliminated by the observation of reflections ($0kl$) with $k+l$ odd, and $T_h^6{-}Pa3$ by ($0kl$) with k odd.

The density 5·95 g.cm.$^{-3}$ reported for a specimen containing 33·0 (wt.) % of silicon (Landolt-Börnstein, 1931, p. 330) leads to 3·86$\sim$4 atoms of iron and 3·86$\sim$4 atoms of silicon in the unit cell. It is assumed that the iron and silicon atoms are distributed in a definite, non-statistical fashion. The final correspondence between calculated and observed structure factors constitutes the ultimate justification of this assumption. (Furthermore, there seems to be no reasonable statistical distribution involving four iron and four silicon atoms for any one of the three possible space groups.)

It is impossible to place four iron and four silicon atoms in sets of equivalent positions of the space groups $T^1{-}P23$ and $T_h^1{-}Pm3$ which are not also equivalent positions of the space group $T_d^1{-}P\bar{4}3m$ (which has the Laue symmetry $O_h{-}4/m\,\bar{3}\,2/m$). The structure must therefore be based on the space group $T^4{-}P2_13$. The observed absence of reflections of the type ($h00$) with h odd is consistent with the choice of this space group. Four iron and four silicon atoms may be placed in sets of equivalent positions in only one manner, namely, in two sets of equivalent positions of the type (x, x, x; $x+\frac{1}{2}, \frac{1}{2}-x, \bar{x}; \cancel{}$).

A set of 15° oscillation photographs about a twofold axis was prepared in a cylindrical camera with a radius of 5 cm. by use of Mo $K\alpha_1$, α_2 radiation filtered by zirconium foil. Three films interleaved with 0·001 in. copper foil were used for each exposure (Hughes, 1941). Intensities of reflections observed in the photographs were estimated visually. Absorption corrections, omitted here, were estimated to be small. The atomic scattering factors for iron were taken as averages between those of Pauling & Sherman (1932) and of Thomas & Fermi (*Internationale Tabellen*...), and the atomic scattering factors for silicon as averages between those of Pauling & Sherman and of James & Brindley (*Internationale Tabellen*...). A temperature factor

exp $[0\cdot5\{(\sin\theta)/\lambda\}^2]$ was applied to calculated structure-factor values.

Table 1. *Intensities of X-ray reflections on oscillation photographs of* FeSi

| (hkl)	Obs.	Calc.	(hkl)	Obs.	Calc.	(hkl)	Obs.	Calc.
110	11	9·5	710	<3·0	3·1	490	3·1	2·5
020	8·8	11	550	4·5	4·6	940	Abs.	1·6
120	13	12	460	7·0	6·6	770	<3·0	2·4
210	26	33	640	6·8	6·6	680	<3·0	1·8
220	2·5	2·7	270	Abs.	0·2	860	<3·0	1·8
130	5·6	4·7	720	5·6	5·9	0.10.0	6·8	5·6
310	5·9	6·9	370	3·3	4·1	1.10.0	3·7	3·1
230	14	13	730	4·2	4·4	10.1.0	3·0	2·2
320	8·4	7·0	560 }	9·1	9·0	2.10.0	Abs.	1·2
040	25	25	650 }			10.2.0	Abs.	1·2
140	Abs.	0·6	080	7·2	6·4	590	<3·0	2·0
410	8·5	10	180	Abs.	1·2	3.10.0	4·1	4·0
330	7·4	6·3	810	6·3	6·4	10.3.0	Abs.	1·8
240	4·6	5·1	470	Abs.	0·9	780	Abs.	1·2
420	4·8	5·1	740	Abs.	0·6	870	Abs.	0·4
340	<1·9	2·3	280	Abs.	0·8	4.10.0	4·9	4·3
430	3·8	3·4	820	Abs.	0·8	10.4.0	4·5	4·3
150	5·9	6·2	660	4·4	4·2	690	6·1	4·5
510	3·9	4·3	380	Abs.	0·7	960	Abs.	1·0
250	18	19	830	<3·0	2·7	1.11.0	3·5	3·4
520	6·5	7·2	570	4·5	4·4	11.1.0	Abs.	0·7
440	16	15	750	Abs.	0·3	2.11.0	Abs.	1·6
350	2·7	3·0	480	5·9	5·2	11.2.0	6·0	4·3
530	3·3	3·2	840	5·7	5·2	5.10.0	Abs.	1·1
060	11	11	190	<3·0	2·4	10.5.0	2·8	2·3
160	5·6	5·8	910	3·1	3·7	880	4·0	2·9
610	8·9	9·9	670	Abs.	1·1	790	Abs.	0·6
260	2·4	2·9	760	6·2	5·2	970	4·5	3·6
620	2·6	2·9	290	8·2	7·7	3.11.0	2·3	2·3
450	7·5	6·9	920	<3·0	2·7	11.3.0	Abs.	1·3
540	<3·0	2·3	580	<3·0	2·0	6.10.0	2·8	2·3
360	5·8	6·3	850	5·8	5·5	4.11.0	Abs.	1·1
630	4·9	5·3	390	Abs.	0·7	11.4.0	Abs.	1·1
170	4·4	4·2	930	4·4	4·2			
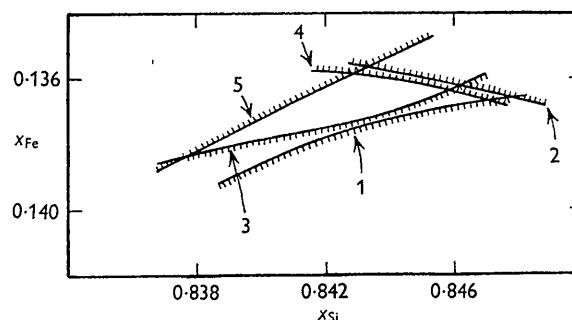
Fig. 1. Determination of parameters.

Curve	Comparison
1	$2F_{10,0,0}^2 < 4F_{1,10,0}^2 + F_{10,0,0}^2$
2	$2F_{10,0,0}^2 > 4F_{10,1,0}^2 + F_{10,0,0}^2$
3	$\|F\|_{920} > \|F\|_{830}$
4	$\|F\|_{850} > \|F\|_{840}$
5	$\|F\|_{4,10,0} > \|F\|_{3,10,0}$

Structure factors calculated with $x_{Fe}=0\cdot1370$ and $x_{Si}=0\cdot8420$ show good agreement with those calculated from the observed intensities (Table 1). Intensity comparisons between reflections having nearly identical angle-dependent factors and observed on the same side of a given film were used to establish the limits of error shown graphically in Fig. 1.† Presumably reliable

* The Mo $K\alpha_1$ components of well-resolved doublets were used for these measurements; the value 0·70926 A. was assumed for λ. It is probable that earlier measurements of a_0 are reported in kX. units. If this is the case, the measurement of the present investigation is in good agreement with the measurements of Phragmén (1923) and Borén (1933).

† Owing to the experimental arrangement the $K\alpha_2$ component of the reflection (10.0.0) was coincident with the $K\alpha_1$ components of the reflections (10.1.0) and (10.1̄.0) on one exposure and the $K\alpha_1$ components of the reflections (1.10.0) and (1̄.10.0) on another exposure. The well-known intensity ratio of the $K\alpha_1$ to the $K\alpha_2$ line, 2 : 1, was used to make the intensity comparisons involving these coincidences shown in Fig. 1.

values of x_{Fe} and x_{Si} are 0.1370 ± 0.0020 and 0.842 ± 0.004, respectively. These are in essential agreement with those of Wever & Moeller (1930) and of Borén (1933).

Discussion of the structure

The interatomic distances

The ligands of each iron atom in FeSi are seven silicon atoms at distances 2·29 A. (1), 2·34 A. (3) and 2·52 A. (3), and six iron atoms at 2·75 A., these distances being reliable to about 0·01 A. The corresponding bond numbers, calculated with the assumption of the normal single-bond radii 1·165 A. for iron and 1·173 A. for silicon (Pauling, 1947), are 1·21, 1·00, 0·50 and 0·20, respectively; the sum of these values for the bonds formed by an iron atom is 6·91, which differs significantly from the expected value 5·78. Each silicon atom is surrounded by seven iron atoms at 2·29 A. (1), 2·34 A. (3) and 2·52 A. (3), and six silicon atoms at 2·78 A., the corresponding bond numbers being 1·21, 1·00, 0·50 and 0·19, and the calculated valence of silicon 6·85, which is very much greater than the normal value 4.

Let us now consider the electronic structure that would be expected for the iron silicide crystal according to the resonating-valence-bond theory of metals (Pauling, 1948). According to this theory, silicon, with only four stable orbitals in its outer shell, could not form more than four electron-pair bonds, which might, however, resonate among more than four positions. In order for metallic resonance of the valence bonds to occur, some of the atoms must possess an extra orbital, the metallic orbital; it is not necessary, however, that the silicon atom itself possess a metallic orbital, inasmuch as its four bonds might undergo pivoting resonance about it, if the surrounding atoms possess the metallic orbital. Moreover, it is to be expected that the resonance of the four bonds of the silicon atom would be of such a nature as to lead to the assignment to the interatomic positions of bond numbers equal to simple fractions, such as $\frac{1}{2}$, $\frac{1}{3}$, $\frac{2}{3}$, ... We note that the observed interatomic distances 2·34 A. (for three bonds) and 2·52 A. (for three) differ by just 0·18 A., which corresponds to a factor $\frac{1}{2}$ in bond number, and that the remaining bond distance, 2·29 A., is slightly smaller (0·05 A.) than the smaller of the other two, suggesting that its bond number is slightly greater. These distances hence suggest that the corresponding bond numbers are 1, $\frac{2}{3}$, and $\frac{1}{3}$, their sum thus being equal to the normal valence 4 for silicon. We assume, as has been found necessary for other crystals also, that the valence of the silicon atom is concentrated entirely into the bonds with its nearest neighbors, and that the six silicon neighbors at 2·78 A. are not bonded by the silicon atoms, the bond number 0·19 given by equation (1) being illusory.

The silicon atom is thus to be described as using one

of its four tetrahedral sp^3 bond orbitals in forming an essentially non-resonating single bond with one iron atom, at 2·29 A.; the other three orbitals resonate between the three iron atoms at 2·34 A., and the three at 2·52 A., the latter set being the less favored, by the factor $\frac{1}{2}$, presumably because of their less satisfactory relation to the tetrahedral directions (the angle with the non-resonating bond being 40° less than the tetrahedral angle, as compared with 26° more for the former set).

When the two longer distances are corrected by 0·11 and 0·29 A. for bond numbers $\frac{2}{3}$ and $\frac{1}{3}$, respectively, and the single-bond radius of silicon is also subtracted, there are obtained the values 1·12, 1·06 and 1·06 A., respectively, for the single-bond radius of iron. Moreover, we expect that the iron atom has the valence 6 (rather than the valence 5·78 found in elementary iron), for reasons described below; of this valence four units are used in bonds with silicon, leaving two valences to be divided among the six iron–iron bonds. The iron–iron distance 2·75 A., when corrected by the amount 0·29 A. corresponding to bond number $\frac{1}{3}$, leads to 1·23 A. for the single-bond radius of iron. These four values show striking deviation from the single-bond radius 1·165 A. found for elementary iron (Pauling, 1947).

However, it is known (Pauling, 1948) that elementary iron represents a resonance average between two valence forms of iron. In one of these, Fe_A, two of the eight outer electrons of the atom are atomic electrons, contributing to the ferromagnetic moment, and the other six are valence electrons. Of the nine stable outer orbitals of the iron atom, two are used for the atomic orbitals, and the remaining seven, d^3sp^3, are for the six valence bonds and the metallic orbital. The metallic orbital accordingly has $\frac{3}{7}$ or 42·9 % d character, on the assumption that the hybrid character of the metallic orbital is the same as that of the bonding orbital. The other kind of iron atoms, Fe_B, contains three atomic electrons in three of the d orbitals, the other six orbitals (d^2sp^3) constituting five bonding orbitals and the metallic orbital. These six orbitals have 33·3 % d character. The ferromagnetic saturation moment, 2·22 magnetons, shows that the structures A and B contribute 78 and 22 %, respectively, to elementary iron, the average amount of d character thus being 39·7 %. The corresponding single-bond radius is 1·165 A. The single-bond radius for sp^3 bonds, with no d character, is found by linear extrapolation (Pauling, 1947) to be 1·481 A. On the assumption (Pauling, 1947, 1948) that there is a linear relation between the single-bond radius formed by a hybrid orbital and the amount of d character, there can be derived the equation

$$R_1(\text{Fe}) = 1.481 - 0.797 \, \delta, \qquad (2)$$

where the symbol δ means the fractional amount of d character in the bond orbital. This leads, for example, to the value 1·138 A. for the single-bond radius of the d^3sp^3 bonds formed by Fe_A, which is sexivalent.

We may now use equation (2) in interpreting the

values 1·12, 1·06, 1·06, and 1·23 A. found for the single-bond radius of iron for the different kinds of bonds formed in the FeSi crystal. Application of equation (2) leads to the values 45, 53, and 31 % d character, respectively, for these bonds. Since there are altogether three d orbitals available for use in the six bond orbitals and the metallic orbital, the difference between 3 and the summed amount of d character for the bond orbitals is the d character of the metallic orbital. This difference is found to be 34 %, an entirely reasonable value.

The state of the iron atom in FeSi may thus be described in the following way. The iron atom is sexi-valent iron, Fe_A. It uses four of its orbitals in forming bonds with the seven surrounding silicon atoms—one single bond, three $\frac{2}{3}$ bonds, and three $\frac{1}{3}$ bonds—and two of the remaining orbitals, and the corresponding valence electrons, in forming six $\frac{1}{3}$ bonds with six neighboring iron atoms. The orbitals involved in the bonds with silicon are different in hybrid character from those involved in the bonds with iron; they have between 45 and 53 % of d character, whereas the bonds with iron have only 31 % d character. The metallic orbital has essentially the same hybrid character, 34% d, as the bond orbital with the smallest d character.

It is interesting to note that the four iron–silicon bond orbitals make use of just two of the three available d orbitals, the third being used by the two bond orbitals involved in iron–iron bonds and the metallic orbitals. Moreover, the distribution of the d orbitals among the orbitals of each class is essentially uniform; the four orbitals involved in bonds with silicon have approximately one-half d character, and the two orbitals involved in iron–iron bonds and the metallic orbital have approximately one-third d character. If it is assumed that the amounts of d character for these classes of orbitals are precisely $\frac{1}{2}$ and $\frac{1}{3}$, respectively, the bond numbers calculated for the four kinds of bonds become 0·85, 0·70, 0·35 and 0·33, respectively, adding up to the valence 6. It is not clear whether the treatment of the distances in which the bond numbers are supposed to be simple (1, $\frac{2}{3}$, $\frac{1}{3}$) or the slightly different treatment in which the amounts of d character are supposed to be simple ($\frac{1}{2}$, $\frac{1}{3}$) is to be preferred.

It has hence been found that the interatomic distances in FeSi are compatible with those in metallic iron and elementary silicon, with the principal difference that the iron atom in FeSi is sexivalent iron, rather than iron with the average valence 5·78, and the effective radius of iron for the different non-equivalent bonds that have formed in FeSi is different because of a difference in the amount of d character. These values of the iron radius are, however, related to that shown in elementary iron, and may be derived from it.

The compounds CrSi, MnSi, CoSi and NiSi were found by Borén (1933) to have the same structure as FeSi, and he reported values for a_0 and for the two atomic parameters differing very little from those for FeSi. The corresponding bond distances are given in

Table 2, together with the single-bond radii of the metallic atoms calculated from them with the same assumption about bond numbers as made above for FeSi. The values for the amount of d character (δ) are also given, as calculated by the following equation (Pauling, 1948):

$$R_1(\delta, z) = 1·825 - 0·043\,z - (1·600 - 0·100\,z)\,\delta. \quad (3)$$

Here z is the atomic number minus 18. It is seen that the amounts of d character lie in the neighborhood of 50 % for the bonds between the metal atom and silicon, and of 30 % for the metal–metal bonds. The values found for the d character of the metallic orbital show rather wide fluctuations, which presumably have little significance. (The magnetic data reported for MnSi, FeSi, and CoSi (Foëx, 1938) are difficult to interpret because of lack of correspondence with the Weiss-Curie equation, and hence are not useful in this case as a criterion of electronic structure.)

Table 2. *Bond distances and bond character in* FeSi *and related crystals*

(All distances in A.)

	M–Si			M–M	Metallic orbital
	1 bond $n=1$	3 bonds $n=\frac{2}{3}$	3 bonds $n=\frac{1}{3}$	6 bonds $n=\frac{1}{3}$	
		CrSi ($a_0=4·620$)			
Bond distance	2·32	2·43	2·58	2·83	
$R(1)$	1·15	1·15	1·12	1·27	
% d character	42	42	45	30	69
		MnSi ($a_0=4·548$)			
Bond distance	2·30	2·39	2·55	2·79	
$R(1)$	1·13	1·11	1·09	1·25	
% d character	43	46	48	30	57
		FeSi ($a_0=4·489$)			
Bond distance	2·29	2·34	2·52	2·75	
$R(1)$	1·12	1·06	1·06	1·23	
% d character	45	53	53	31	34
		CoSi ($a_0=4·438$)			
Bond distance	2·28	2·33	2·47	2·73	
$R(1)$	1·11	1·05	1·01	1·22	
% d character	47	56	61	31	18
		NiSi ($a_0=4·437$)			
Bond distance	2·28	2·33	2·47	2·73	
$R(1)$	1·11	1·05	1·01	1·22	
% d character	47	57	64	29	17

The choice of the FeSi *structure*

Some general considerations about the selection of the FeSi structure by iron silicide and related substances may now be formulated. It is clear that the sodium chloride structure would not be a satisfactory one—in this structure an atom has as its neighbors only six atoms of the other kind, all more distant neighbors being so far removed as not to permit the formation of a significant bond with them; the effective valences of the two kinds of atoms are hence the same, and the structure is accordingly an unsuitable one for two elements with such different valences as 4 and 6. On the other hand, the nickel arsenide structure, with

small axial ratio, such as shown by AuSn (Pauling, 1947), might be assumed by FeSi. The axial ratio could adjust itself in such a way that the silicon atom would use its valence of 4 in forming four bonds with the surrounding six iron atoms, and the iron atom would use its extra valence 2 in forming two iron–iron single bonds, one with each of the iron atoms above and below it along the c axis. Similarly, the cesium chloride structure might be assumed by FeSi, each silicon atom then forming eight half-bonds with the iron atoms surrounding it in a cubic arrangement, and each iron atom forming eight half-bonds with silicon atoms, and six one-third bonds with the six adjacent iron atoms. It seems not unlikely that co-ordination number 6 (bond number $\frac{2}{3}$) is more suitable for silicon in an inter-metallic compound than co-ordination number 8* (bond number $\frac{1}{2}$), and that, moreover, resonating iron–iron bonds, with bond number $\frac{1}{3}$, are more stable than non-resonating bonds, with bond number 1. The actual FeSi structure would thus be preferred to the cesium

chloride structure for the first reason, and to the nickel arsenide structure for the second reason.

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* A substance in which the four bonds of the silicon atom show pivoting resonance among eight positions is Mg_2Si, with the fluorite structure (Pauling, 1948).

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Atomic Displacements in the Austenite–Martensite Transformation

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The atomic displacements in the transformation from austenite to martensite are described, and the strains involved are derived. It is shown that the tetragonality of martensite arises as a necessary consequence of the assumption that the iron and carbon atom displacements constitute a common homogeneous deformation. An explanation of the observed high indices of the habit plane of martensite of certain carbon contents is advanced.

1. Introduction

The transformation from austenite to martensite is an example of a phase change occurring, not by the usual nucleation and growth processes, but by a homogeneous deformation of the crystal structure of the original phase to produce that of the final phase. The characteristics of transformations of this kind are that, immediately the appropriate conditions (temperature, pressure, etc.) are set up, discrete macroscopic regions of the original structure deform by an *Umklappung* or 'clicking-over' process and the new structure is established. From the point of view of visual observation the phase change of any individual transformation unit occurs instantaneously, although the deformation must presumably propagate through the region at a finite speed. Mechanical twinning is an

example of a phase change of this general type, the special characteristic of which is that the original and final structures differ only in orientation.

Austenite and martensite are essentially dilute interstitial solutions of carbon in the face-centred cubic and body-centred cubic forms of iron respectively. The transformation from austenite to martensite is therefore best discussed by considering first a hypothetical similar transformation between the corresponding phases in pure iron, and then dealing separately with the slight modifications caused by the dissolved carbon atoms. It should be emphasized that this treatment is adopted for theoretical simplicity only, and that the corresponding phase transformation in pure iron does not occur by a deformation process but by nucleation and growth.