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The Crystal Structure of Mn_5Si_2 and the *D* Phase (V–Fe–Si)*

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The structure model derived earlier for the *D* phase, $V_{26 \cdot 5}Fe_{44}Si_{29 \cdot 5}$, has been refined by full-matrix least squares with diffractometer data for the isotypic Mn_5Si_2. Mn_5Si_2 is tetragonal, $a = 8 \cdot 9097 \pm 2$, $c = 8 \cdot 7153 \pm 3$ Å, 56 atoms per unit cell, space group $P4_12_12$. The final $R(F)$ for the refinement with isotropic thermal parameters is 0·082 (all 640 independent reflections), or 0·053 (463 reflections with $I > 2\sigma$). The structure belongs to the family of σ-phase related phases; it is 'tetrahedrally close packed' (t.c.p.), but it has four-coordinated bonds in addition to the five- and six-coordinated bonds found in 'ideal' t.c.p. structures. The structure does not possess non-tetrahedral interstices as does α-Mn (*A*12), which possesses distorted octahedral interstices. Mn and Si appear to be ordered: of the 56 atoms in the unit cell, sixteen (29%) have CN 16 (Mn), eight (14%) have CN 14 (Mn), sixteen (29%) have CN 12 (eight Mn, eight Si), eight (14%) have CN 13 (Mn) and eight (14%) have CN 11 (Si). Unlike the ν phase ($Mn_{81 \cdot 5}Si_{18 \cdot 5}$), this structure possesses some Si–Si bonds.

Introduction

A phase of composition Mn_5Si_2 was indexed on a tetragonal cell by Sénateur & Fruchart (1964); this apparently is one of the 'low-temperature' (~600°C) phases mentioned by Åmark, Borén & Westgren (1936). The *D* phase was discovered by Bardos & Beck (1966) in the V–Fe–Si and the V–Mn–Fe–Si systems and indexed on a similar tetragonal cell. Setz, Nowotny & Benesovsky (1968) suggested that Mn_5Si_2 and the *D* phase are isotypic; this was confirmed by Shoemaker & Shoemaker (1971*c*) by a careful comparison of the powder diffraction diagrams. A specimen of the *D* phase of composition $V_{26 \cdot 5}Fe_{44}Si_{29 \cdot 5}$ was kindly made available to us by Professor Paul A. Beck, University of Illinois. Some years ago we derived a model for the structure, although the single crystals isolated were very small and badly twinned and only about 50 independent reflections were obtained on Weissenberg pictures taken with Cr $K\alpha$ radiation (Shoemaker & Shoemaker, 1965, 1966). We now report a refinement of this structure model with diffractometer data obtained from a single crystal isolated from a sample of Mn_5Si_2, kindly sent to us by Dr R. Fruchart, Institut National Polytechnique de Grenoble, France.

Experimental

The cell dimensions listed in Table 1 were determined by least squares from powder diffraction diagrams taken with Fe $K\alpha_1$ radiation (Sénateur, Fruchart & Shoemaker, 1975). Intensity data for a crystal fragment in arbitrary orientation were collected on a Syntex $P\bar{1}$ diffractometer with Mo $K\alpha$ radiation and a graphite monochromator. A θ–2θ scan was used and all reflections in one octant of reciprocal space out to $2\theta = 60°$ were measured. The scan rate was 1 deg min^{-1}; the 2θ range was 1·6° plus the $\alpha_1\alpha_2$ angular separation. Background readings were made at the beginning and the end of each scan range; the background time/scan time was unity. A total of 1200 reflections were measured, of which 640 were independent. The crystal fragment was irregularly shaped with dimensions varying between 0·055 and 0·065 mm. An absorption correction was applied assuming spherical shape with $\mu r = 0 \cdot 57$, corresponding to absorption factors ranging from 2·23 to 2·18. In a later stage of the refinement a secondary extinction correction factor of the form $F_o^{corr} = F_o(1 + gI_o)$ (Zachariasen, 1963) was applied. The real part of the anomalous dispersion correction (Cromer, 1965) was included, and the imaginary part was used at the end of the refinement to distinguish between the two possible enantiomorphous space groups.

Table 1. *Crystal data for* Mn_5Si_2

F.W. 330·36
$a = 8 \cdot 9097 \pm 2$ Å
$c = 8 \cdot 7153 \pm 3$
$V = 691 \cdot 84 \pm 5$ Å^3
λ (Fe $K\alpha_1$) = 1·93597 Å
μ (Mo $K\alpha$) = 189·6 cm^{-1}

Space group: $P4_12_12$ (D_4^4)
$Z = 56$ atoms/cell
$D_m = 6 \cdot 34 \pm 2$ g cm^{-3}
$D_x = 6 \cdot 343$
$F(000) = 1240$

Structure model

The structure is tetragonal, Laue group $4/mmm$, with systematic extinctions: $h00$ with h odd, $00l$ with $l \neq 4n$, corresponding to space group $P4_12_12$ and its enantiomorph $P4_32_12$. The structure model for the *D* phase, $V_{26 \cdot 5}Fe_{44}Si_{29 \cdot 5}$ (Shoemaker & Shoemaker, 1965, 1966), was used; this model was derived from the resemblance of certain features of the diffraction pattern to those of the σ phase (Bergman & Shoe-

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maker, 1954). The cell dimensions of the *D* phase are very similar to those of the σ phase, except for a doubling of the *c* axis. Both structures are tetragonal and the number of atoms per unit cell in the *D* phase (56) is almost twice that for the σ phase (30). The *hk*0 reciprocal layer of the *D* phase resembles that of the σ phase, indicating that σ-phase type layers (consisting of hexagons and triangles, with the hexagons in successive layers antisymmetrically superimposed in the σ phase itself) occur in the *D* phase perpendicular to the *c* axis. The cell dimensions of the *D* phase are quite similar to those for the δ phase (Shoemaker & Shoemaker, 1963) and for both structures the number of atoms per unit cell is 56. The δ phase is, however, only pseudo-tetragonal (its actual space group is $P2_12_12_1$) and it contains puckered σ-phase type layers perpendicular to the *a* and *b* axes.

The three-dimensional Patterson function calculated for the *D* phase confirmed the presence of puckered σ-phase type layers perpendicular to the *c* axis but had in addition a very high peak at $0{\cdot}20,0,\frac{1}{2}$. This peak was interpreted to indicate that σ-phase layers $c/2$ apart are shifted by $0{\cdot}20,0,\frac{1}{2}$. This arrangement was achieved by placing a σ-phase layer at $z\sim 0$, with the atom that is at the origin of the σ phase located at $x,y=0{\cdot}10,0$ with respect to a 4_1 axis. The 2_1 axes parallel to *a* are in the same positions as the 2_1 axes between the layers in the σ phase. The 2_1 axes parallel to *b* require a puckering of the layers. It appeared possible to pucker the layers by trial so that good coordinations were obtained for some of the atoms, and four atoms per unit cell were eliminated by fusion. This structure model was refined by least squares, but good agreement could not be obtained because of the very limited and imprecise data set (50 observed reflections out of a possible 150 with Cr $K\alpha$ radiation).

Structure refinement

Data treatment

The trial structure was successfully refined with the data set obtained as described above for a crystal of Mn_5Si_2. The data reduction and the initial refinement cycles were done on Oregon State University's CDC 3300 computer with local versions of the programs *STUDIT*, *INCOR* (Zalkin), *SUFLS* (based on the Oak Ridge least-squares refinement program) and *LSLONG* (based on Zalkin's modification of the Gantzel–Sparks–Trueblood refinement program). The *hkl* and *khl* data were averaged and the scattering factors for the neutral atoms were taken from *International Tables for X-ray Crystallography* (1962) and corrected for the real part of the anomalous dispersion (Cromer, 1965) with $f'=0{\cdot}36$ for Mn and 0·09 for Si. The weights were based on the standard errors in the averaged intensities I_o calculated with the equation $\sigma(I_o)=0{\cdot}786[C+B+(0{\cdot}05C)^2+(0{\cdot}05B)^2]^{1/2}$. (*C* is the count integrated over the diffraction maximum, *B* is the total background count. The factor 0·786 is calculated by the program *STUDIT* to bring the σ's into agreement, on the average, with those calculated from the scatter of the data; the factor 0·05 in the formula is evidently too large.) All reflections were used in the refinement; the reflections with intensities lower than the background were entered with a very small positive value; for such reflections we arbitrarily assumed $\sigma(F)=[\sigma(F^2)]^{1/2}$. The final refinement cycles were performed on the Lawrence Berkeley Laboratory CDC 7600 computer from a remote terminal with the *LESQ* program contained in Zalkin's X-RAY 76 program system. In these cycles absorption, extinction and anomalous-dispersion corrections were applied.

Ordering of the atoms

In the original model we assumed that the positions with irregular coordinations, which later turned out to have CN 11 and 13, were occupied by Si and the positions with CN 12, 14 and 16 by Mn. Variation of the occupancies, while keeping the isotropic *B* parameters fixed at an average value, indicated that the CN 13 position was actually occupied by Mn and that the Si atoms occupied the position with CN 11 and one of the positions with CN 12. This distribution was assumed in the final cycles and led to a reasonably limited spread in the thermal parameters. From this we conclude that Mn and Si in Mn_5Si_2 are fully ordered (apart from possible admixtures of less than 5 at.%), in contrast to our findings for the ν phase ($Mn_{81\cdot5}Si_{18\cdot5}$, Shoemaker & Shoemaker, 1971*a*), where some CN 12 positions are solely occupied by Mn or Si, but where other CN 12 positions contain various mixtures of Mn and Si.

Thermal and positional parameters

First attempts to vary the isotropic *B* parameters led to negative values for all atoms. Application of extinction and absorption corrections (see under *Experimental*) gave the final isotropic *B* values listed in Table 3 and agreement indices listed in Table 2. Two more cycles were run with anisotropic thermal parameters. Application of the significance test (Hamilton, 1965) to the R_w values (Table 2) shows that 'the hypothesis of isotropic motion can be rejected at the 0·005 level'. Analysis of the thermal ellipsoids shows, however, that for all atoms the mean square displacement along **c** is about $\frac{2}{3}$ of the displacements along **a** and **b**, which do not differ significantly from each other. Atom Si(6) has a very small displacement in the **c** direction. Therefore the anisotropic thermal parameters probably do not have physical meaning in terms of anisotropic thermal motion. Rather they may reflect the inadequacy of the spherical absorption correction; an ellipsoid may be a better approximation for the shape of the crystal. The positional parameters listed in Table 3 were obtained at the end of the refinement with anisotropic thermal parameters. They differ by less than σ from the values obtained at the end of the isotropic refinement [except a difference of 1·5σ in the y parameter for Si(8)].*

Table 2. *Agreements obtained in the least-squares refinements of* Mn_5Si_2

$$\Delta F = ||F_o| - |F_c||.$$
$$R = \sum \Delta F / \sum |F_o|,\ R_w = \{\sum[w(\Delta F)^2] / \sum[wF_o^2]\}^{1/2}.$$
$$S = \{\sum[w(\Delta F)^2]/(NO - NV)\}^{1/2}.$$

	NO	*NV*	*R*	R_w	*S*
hkl and *khl* averaged					
Isotropic	640	29	0·0823	0·0457	1·402
Isotropic, $I > 2\sigma$	463		0·0535		
Anisotropic	640	63	0·0766	0·0408	1·289
Non-averaged data					
x,y and 4_1, isotropic	1196	29	0·1074	0·0459	1·514
y,x and 4_3, isotropic	1196	29	0·1098	0·0477	1·572

Anomalous dispersion

The *hkl* and *khl* data are related as Bijvoet pairs. All data in one octant were measured and in the refinements with the *hkl* and *khl* data averaged only f' was included in f. Two isotropic refinement cycles were run with intensities not averaged for *hk* and *kh* and with f'' included in the scattering factors. (The values used were 0·80 for Mn and 0·09 for Si; Cromer, 1965.) In this refinement the 20 positional parameters changed from the values given by the isotropic refinement by amounts most of which were smaller than σ; one [again y for Si(8)] changed by 2·2σ. The enantiomorph is obtained by interchanging the x and y parameters of the atoms and replacing the 4_1 screw axis by a 4_3 screw axis. Two isotropic cycles were run for the enantiomorph and the agreement indices obtained are compared in Table 2. Although the difference is small, the significance test (Hamilton, 1965) shows that the model with the 4_3 axis may be rejected for the particular crystal specimen used at the 0·005 significance level. The correctness of the 4_1 enantiomorph was also indicated by structure-factor comparisons: for 22 *hkl*–*khl* pairs with calculated structure-factor differences of the order of σ or larger, the observed structure-factor differences were in sign agreement with the 4_1 enantiomorph in 20 cases and with the 4_3 enantiomorph in two.

Description of the structure

The σ-phase nets

Fig. 1 is a stereo view in the **c** direction of part of the structure of Mn_5Si_2 produced by the computer program *ORTEP* (Johnson, 1965). Three puckered nets, related by the operation of 4_1 axes [located between atoms Mn(7)] are shown and the atoms have been connected so as to make these nets resemble the planar nets occurring in the main layers of the σ phase. Atoms Mn(2) and Mn(3) correspond to the atoms in the subsidiary layers of the σ phase which center in projection the hexagons in the main layers. However, the nets in Mn_5Si_2 are so severely puckered that the distinction between main and subsidiary layers has largely lost its meaning and one can connect different sets of atoms to produce σ-phase type nets. The nets in Mn_5Si_2 do not stack in perfect σ-phase fashion. The atoms between the layers in the σ phase are at the centers of hexagonal antiprisms with two polar atoms, resulting in CN 14 coordinations. Atom Mn(2) in Mn_5Si_2 has CN 16: the hexagon formed by atoms Mn(5), Mn(7), Si(6), Si(6), Mn(7), Mn(5) is almost planar, but the hexagon formed by atoms Mn(4), Si(8), Mn(7), Mn(5), Mn(1), Si(6) is somewhat puckered and at the other side of it are three atoms [Mn(1), Si(8) and Mn(3)] neighboring atom Mn(2). Atom Mn(3) (on a diagonal twofold axis) is at the center of gravity of the surrounding puckered hexagon and thus could have been chosen as part of the main layer. Its CN is 14, but the planar hexagons are approximately parallel to **c** [each composed of atoms Mn(1), Si(8), Mn(2), Mn(4), Mn(5), Si(6), with two other atoms Mn(1) as polar atoms]. Fig. 1 also shows the apparent shift of the σ-phase type layers separated by $c/2$ over approximately $\Delta x = 0{\cdot}20$, $\Delta y = 0$ [the horizontal component of the vector between atoms Mn(7) on the two layers] which causes the high peak in the Patterson function used in the derivation of the structure.

The coordination polyhedra and interstices

Mn_5Si_2 and the *D* phase differ in some respects from the 'ideal' tetrahedrally close-packed (t.c.p.) structures (Shoemaker & Shoemaker, 1971*b*): in addition to the

Table 3. *Atomic parameters for* Mn_5Si_2

Positional parameters are from anisotropic refinement; *B* values are from prior isotropic refinement.

CN	Atom	Site	*x*	*y*	*z*	*B* (Å^2)
16	Mn(1)	8(*b*)	0·42038 ± 27	0·18554 ± 28	0·32968 ± 23	0·634 ± 37
16	Mn(2)	8(*b*)	0·17466 ± 29	0·22408 ± 28	0·15031 ± 25	0·831 ± 38
14	Mn(3)	4(*a*)	0·13799 ± 28	0·13799	$\frac{1}{2}$	0·692 ± 56
14	Mn(4)	4(*a*)	0·45162 ± 28	0·45162	$\frac{1}{2}$	0·718 ± 56
12	Mn(5)	8(*b*)	0·36946 ± 26	0·45348 ± 26	0·21380 ± 25	0·484 ± 34
12	Si(6)	8(*b*)	0·46925 ± 52	0·26766 ± 49	0·04582 ± 45	0·480 ± 66
13	Mn(7)	8(*b*)	0·39882 ± 26	0·01027 ± 27	0·07580 ± 23	0·673 ± 34
11	Si(8)	8(*b*)	0·38473 ± 53	0·19232 ± 52	0·60242 ± 42	0·597 ± 65

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31696 (4 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

'normal' coordination numbers of 12, 14 and 16, coordinations of 11 and 13 occur. The CN polyhedra, produced by the program *ORTEP* (Johnson, 1965), are shown in Figs. 2–5, in which Mn atoms are represented by large circles and Si atoms by small circles (although the distances indicate that Mn and Si with the same CN display approximately the same radius). Fig. 2 shows the CN 16 polyhedra for atoms Mn(1) and Mn(2). For both atoms the polyhedra are oriented with an approximate threefold axis in the vertical direction. Fig. 3 shows the CN 14 polyhedra for atoms Mn(3) and Mn(4). These atoms are on twofold axes, which in both figures are approximately horizontal. The approximate sixfold axes are vertical. Fig. 4 shows the CN 12 polyhedra for atoms Mn(5) and Si(6), which are distorted icosahedra. In both cases there is an approximate fivefold axis in the vertical direction. The irregular coordinations are shown in Fig. 5: a CN 13 polyhedron for Mn(7) and a CN 11 polyhedron for Si(8). The CN 13 polyhedron may be considered as an intermediate between an icosahedron (CN 12) and a CN 14 polyhedron: the bond between atom Mn(7) and atom Mn(2) at the bottom is sixfold, but the bond between atom Mn(7) and atom Si(6) at the top of the figure is fivefold. A similar coordination is found in α-Mn (Oberteuffer & Ibers, 1970). The CN 11 polyhedron may be considered as a distorted icosahedron. The bonds between Si(8) and atom Mn(2) in front, and between Si(8) and Mn(3) at the back are both surrounded by pentagons, but these two pentagons share

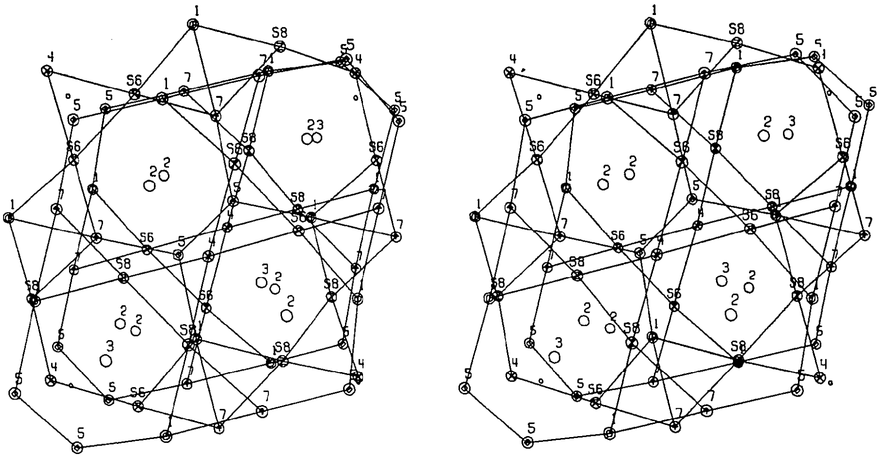


Fig. 1. Stereoscopic view produced by *ORTEP* of part of the structure of Mn_5Si_2 in the direction of the $-c$ axis. The origin is in the lower left-hand corner, a is horizontal, b vertical. The layers at $z\sim0$, $\frac{1}{4}$ and $\frac{1}{2}$ are shown. These layers are related by the operations of 4_1 axes, coincident with the axes of helices of bonded Mn(7) atoms. Here and in Fig. 7 Mn atoms are indicated by their assigned numbers and Si atoms are indicated by their assigned numbers preceded by S.

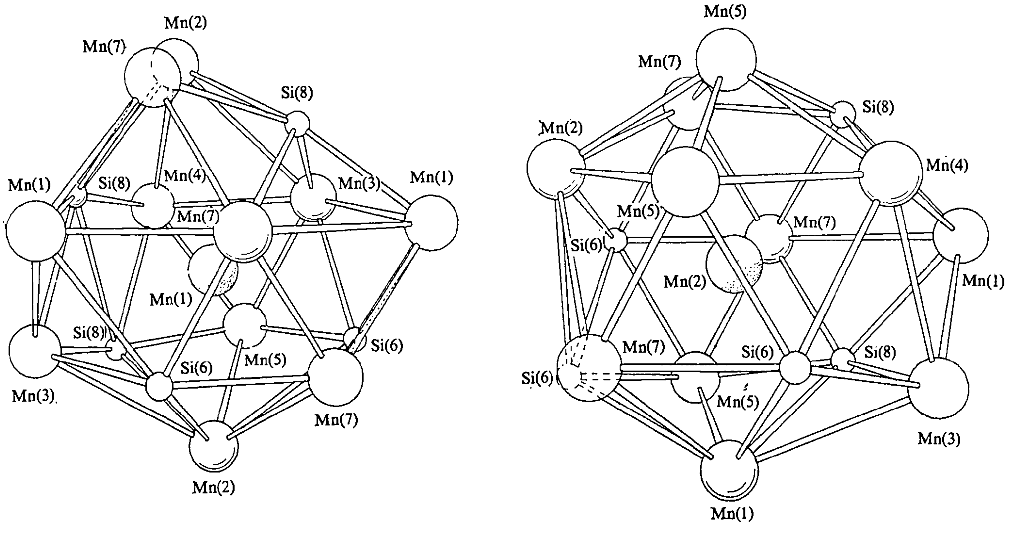


Fig. 2. CN 16 polyhedra of atoms Mn(1) (left) and Mn(2) (right) in Mn_5Si_2.

atom Mn(1) at the bottom of the figure. This type of coordination occurs also for Si in Mn_5Si_3 ($D8_8$ type).

All bonds in t.c.p. structures in which all atoms have one of the 'normal' coordination polyhedra (CN 12, 14, 15 or 16) are five- or six-coordinated. The occurrence of the polyhedra CN 11 and CN 13 in Mn_5Si_2 results in the presence of some four-coordinated bonds. These are shown in Fig. 6. Although one might consider the interstices enclosed by the atoms in Fig. 6 as squashed octahedra, they are better described as four tetrahedra sharing a central edge [Si(8)–Si(8) and Si(8)–Mn(7), respectively] since the lengths of the edges of these tetrahedra are within the limits for those found in the other t.c.p. structures (Shoemaker & Shoemaker, 1969). The coordination polyhedra in Mn_5Si_2 are completely interpenetrating (as defined by Brandon, Chieh, Pearson & Riley, 1975). In this the *D*-phase structure differs from structures like the γ-brasses and α- and β-Mn, which have also been described in terms of tetrahedral interstices, but with some arbitrariness or 'freedom' in the choice of tetrahedra in certain regions of those structures (Brandon *et al.*, 1975).

Interatomic distances and major networks

The interatomic distances are given in Table 4. The range they cover is 2·319–3·364 Å, which is comparable with that in the ν phase, $Mn_{82}Si_{18}$, namely 2·211–3·279 Å (Shoemaker & Shoemaker, 1971*a*) and somewhat larger than that in α-Mn, namely 2·258–2·930 Å (Oberteuffer & Ibers, 1970). As in other t.c.p. structures,

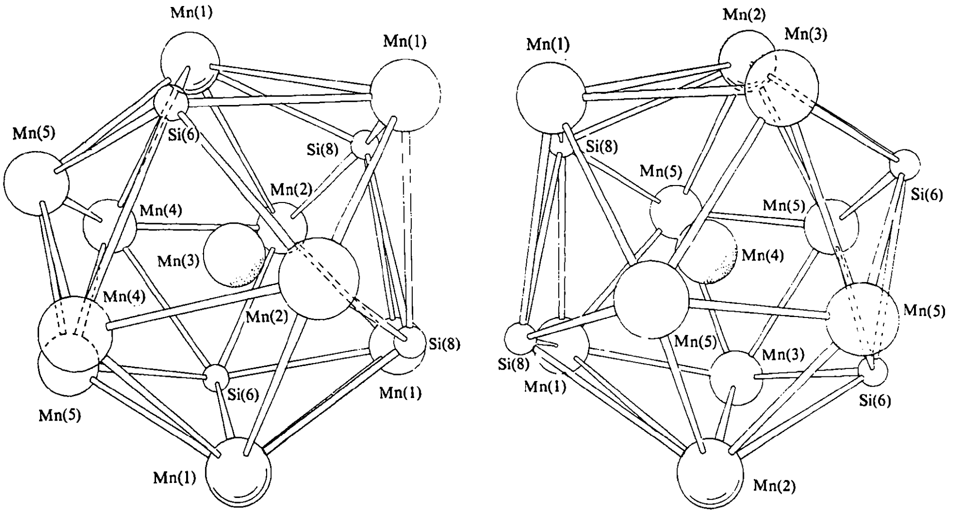


Fig. 3. CN 14 polyhedra of atoms Mn(3) (left) and Mn(4) (right) in Mn_5Si_2.

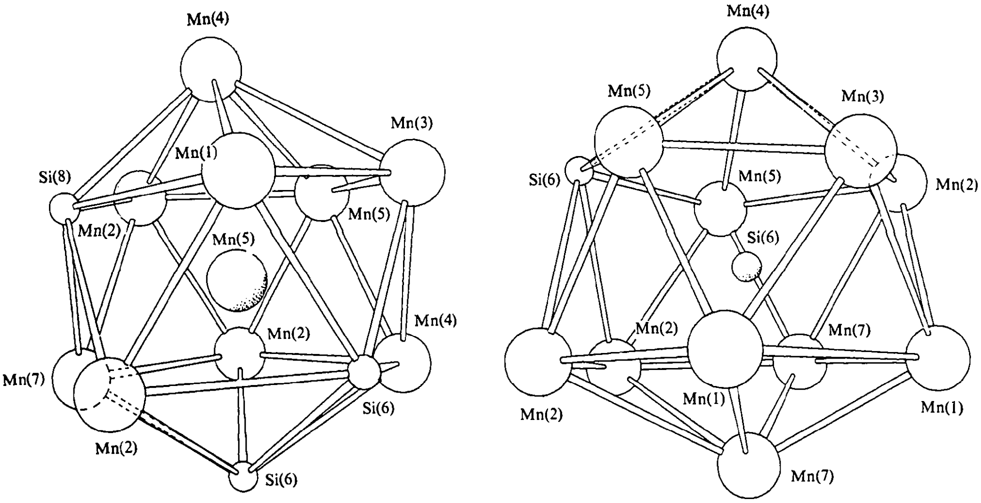


Fig. 4. CN 12 polyhedra of atoms Mn(5) (left) and Si(6) (right) in Mn_5Si_2.

major bonds (those coordinated by six atoms) can be identified and are marked with asterisks in Table 4; four-coordinated bonds are marked with primes. In the ideal t.c.p. structures the major bonds form continuous networks in one, two or three dimensions. In Mn_5Si_2 the major bonds form two interlocking non-interconnected three-dimensional networks (Fig. 7). Unusual about these networks is that atom Mn(7) (CN 13) is connected in its network by two bonds enclosing an angle of 118° and that atom Si(8) (CN 11) is connected to it by only one bond. This last bond, Mn(1)–Si(8), has a distance of 2·399 Å, which is very short for a major bond to a CN 16 atom. However, in ideal t.c.p. structures the atoms in the major networks have CN ≥ 14; Si(8), with only CN 11, may be expected to display a smaller radius.

The distortion of the major network is also demonstrated by the major-bond 'tetrahedral angles' at the CN 16 atoms, which vary between 106·0 and 117·4°, except that the angle CN13–CN16–CN11 is only 93·9°. The angles between the major bonds to the CN 14 atoms, Mn(3) and Mn(4), are 168·5 and 167·2°, respectively (ideally 180°).

The silicon atoms

It has been shown that the stability ranges of t.c.p. structures can in certain cases be extended by the addition of silicon. Bardos, Malik, Spiegel & Beck (1966) and Kuzma & Hladyshevskii (1964) have found that in the Mn–Si system at 1000°C β-Mn dissolves up to 14 at.% Si and at 600°C α-Mn also dissolves 14 at.%. The structures of α- and β-Mn are not t.c.p. but contain many tetrahedral interstices.

With increasing Si in the Mn–Si system two t.c.p. structures appear: at 14·3 at.% Si an *R* phase (Mn_6Si) and at 18 at.% Si the ν or *N* phase ($Mn_{81.5}Si_{18.5}$). The ordering of the atoms has not been investigated in this *R* phase; in the ν phase we found (Shoemaker &

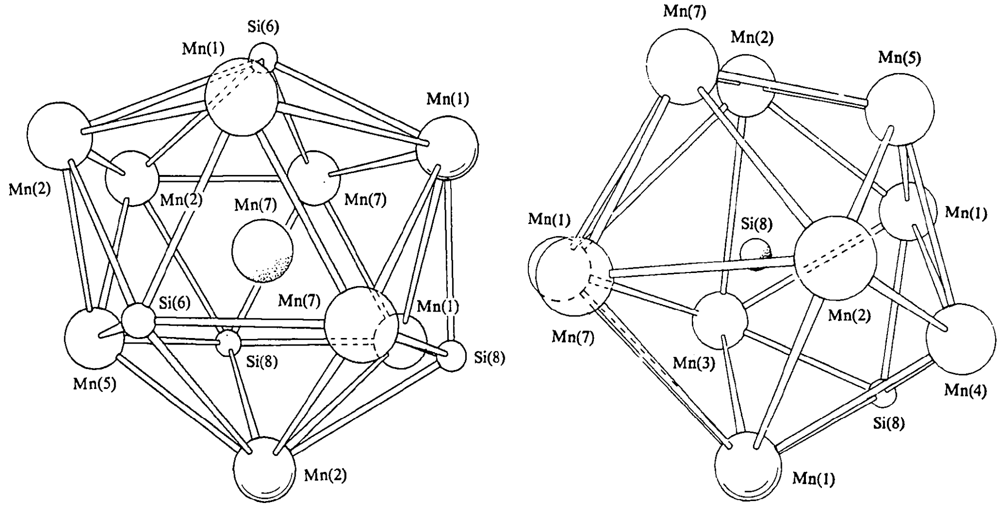
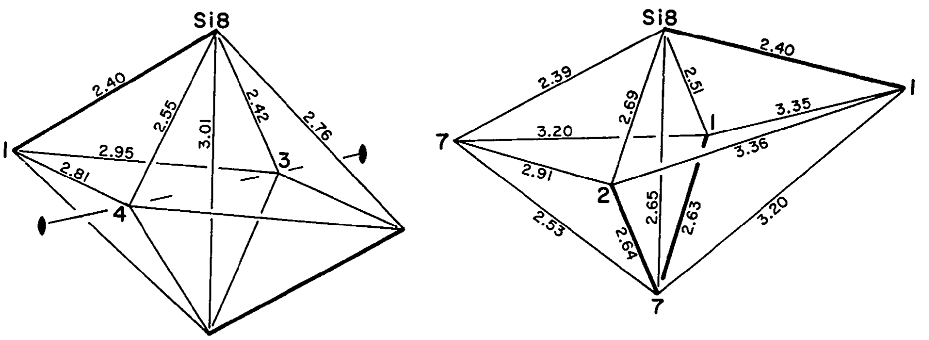


Fig. 5. CN 13 polyhedron of atom Mn(7) (left) and CN 11 polyhedron of atom Si(8) (right) in Mn_5Si_2.



(*a*) (*b*)

Fig. 6. The four-coordinated bonds in Mn_5Si_2. (*a*) Si(8)–Si(8); (*b*) Si(8)–Mn(7). Heavy lines indicate major (six-coordinated) bonds.

Shoemaker, 1971*a*) that essentially all positions with CN > 12 are occupied by Mn and that the CN 12 positions are occupied by mixtures of Mn and Si atoms, except three positions which are occupied by Mn only and two positions which are occupied by Si only. The latter positions have only Mn atoms in their first coordination shells; this was taken as an indication that some charge transfer may occur from Mn to Si. We now find that in Mn_5Si_2, which contains more silicon and is not 'ideally' t.c.p., some Si–Si contacts do occur, namely a Si(6)–Si(6) distance of 2·663 and a Si(8)–Si(8) distance of 3·011 Å.

The structure of β-Mn is stabilized by C atoms and so is the structure of Mn_5Si_3 ($Mn_{62}Si_{38}$, $D8_8$ type). Both structures contain octahedral interstices surrounded by Mn atoms; these interstices are the sites for the C atoms. On the other hand, Sénateur, Spinat & Fruchart (1965) have found that Mn_5Si_2 does not dissolve C

Table 4. *Interatomic distances for* Mn_5Si_2 (Å)

The standard deviations are estimated to range between 0·004 and 0·008 Å. Distances occurring twice when reading down are underlined. Asterisks indicate major bonds; primes indicate four-coordinated bonds.

	CN	Mn(1) 16	Mn(2) 16	Mn(3) 14	Mn(4) 14	Mn(5) 12	Si(6) 12	Mn(7) 13	Si(8) 11
Mn(1)	16	3·350	2·712* 3·364	2·591* 2·952	2·811	2·632	2·571 2·616	2·628* 2·715 3·200	2·399* 2·510 2·762
Mn(2)	16	2·712* 3·364	2·693*	3·160	2·675*	2·637 2·687 2·738	2·651 2·805 2·895	2·641* 2·835 2·907	2·592 2·689
Mn(3)	14	2·591* 2·952	3·160		2·853	2·547	2·477		2·422
Mn(4)	14	2·811	2·675*	2·853		2·594 2·600	2·629		2·547
Mn(5)	12	2·632	2·637 2·687 2·738	2·547	2·594 2·600	2·319	2·382 2·442	2·468	2·331
Si(6)	12	2·571 2·616	2·651 2·805 2·895	2·477	2·629	2·382 2·442	2·663	2·392 2·452	
Mn(7)	13	2·628* 2·715 3·200	2·641* 2·835 2·907			2·468	2·392 2·452	2·528	2·388 2·652′
Si(8)	11	2·399* 2·510 2·762	2·592 2·689	2·422	2·547	2·331		2·388 2·652′	3·011′

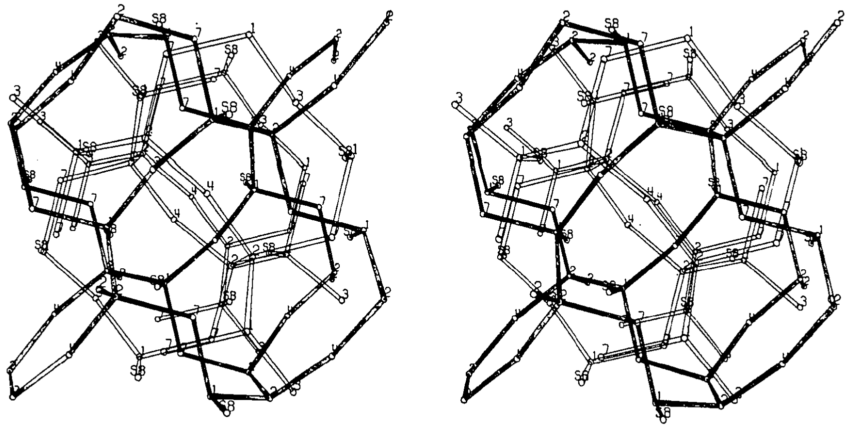


Fig. 7. Stereoscopic view produced by *ORTEP* of the two interpenetrating 'major networks' of six-coordinated bonds in Mn_5Si_2 in the direction of the $-c$ axis.

atoms. Carbon-containing phases have been identified in the Mn–Si systems at approximate compositions Mn_5SiC and Mn_4SiC and their structures have been determined (Spinat, Fruchart, Kabbani & Herpin, 1970; Spinat, Brouty, Wheeler & Herpin, 1975). They are somewhat related to the t.c.p. structures, but they contain trigonal prisms of Mn atoms in which carbon atoms are located.

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