XXXVI. The Crystal Structure of Cementite.

By

Sterling B. Hendricks in Washington.

(With 3 figures.)

Cementite, Fe_3C, is the only described carbide of iron now recognized as a component of the iron carbon system. **Westgren** and **Phragmén**[1]) have made a series of powder, Laue and rotating crystal photographs from crystals of cementite containing some manganese. Cohenite, meteoric iron carbide containing some nickel, was shown to give powder photographs similar to those of cementite. From their examination of the data obtained they concluded that the crystals are orthorhombic and that the dimensions of the unit of structure containing $4Fe_3C$ are 4.518 Å × 5.069 Å × 6.736 Å. The published data are extensive enough to allow a complete structure determination to be carried out.

Experimental Data.

In the determination of the crystal structure of Fe_3C it was necessary to use only the data from rotating crystal photographs listed by **Westgren** and **Phragmén**. These data are here listed as Tables I, II and III. Their photographs were made with iron K radiation. A tabular crystal was used that had somewhat irregular spacial extension. This latter fact must be borne in mind in evaluating intensities of reflection.

Photographs were made in this laboratory from crystals of cohenite kindly given to me by the late Dr. **Merrill** of the United States National Museum and from crystals of cementite that Professor **Westgren** of the Stockholm Högskola, kindly sent to me. Powder photographs were made from pure Fe_3C. The resulting data are essentially the same as those obtained by **Westgren** and **Phragmén**.

I. Unit of Structure.

a) Symmetry. Orthorhombic. Determined from Laue photographs of cementite and of cohenite.

b) Dimensions $a = \mathbf{4.51_8}$ Å
$b = \mathbf{5.06_9}$ Å
$c = \mathbf{6.73_6}$ Å.

---

1) A. **Westgren** and G. **Phragmén**, J. Iron Inst. **105**, 241. 1922; **109**, 159. 1924.

Table I.

Photograph I. Rotation Axis Parallel to the Shortest Edge (a_1) of the Elementary Parallelepiped (Westgren and Phragmén).

I	$h_1h_2h_3$	R	I	$h_1h_2h_3$	R	I	$h_1h_2h_3$	R
v. w.	002	$K\alpha$	w.	112	$K\alpha$	w.	210	$K\beta$
v. w.	021	$K\beta$	v. w.	121	$K\beta$	w.	211	$K\beta$
m.	021	$K\alpha$	w.	120	$K\alpha$	s.	211	$K\alpha$
w.	022	$K\beta$	w.	103	$K\beta$	w.	202	$K\alpha$
s.	022	$K\alpha$	m.	121	$K\alpha$	w.	212	$K\alpha$
w.	$\left\{\begin{matrix}004\\023\end{matrix}\right\}$	$K\beta$	s.	103	$K\alpha$	s.	212	$K\beta$
m.	$\left\{\begin{matrix}004\\023\end{matrix}\right\}$	$K\alpha$	m.	113	$K\alpha$	w.	221	$K\alpha$
w.	025	$K\beta$	w.	122	$K\alpha$	w.	222	$K\alpha$
m.	006	$K\beta$	m.	130	$K\alpha$	w.	223	$K\alpha$
w.	043	$K\beta$	w.	131	$K\alpha$	w.	233	$K\beta$
s.	025	$K\alpha$	w.	114	$K\alpha$	w.	215	$K\alpha$
v. w.	042	$K\alpha$	w.	124	$K\alpha$	w.	232	$K\alpha$
s.	006	$K\alpha$	w.	105	$K\alpha$	v. w.	224	$K\alpha$
s.	043	$K\alpha$	w.	$\left\{\begin{matrix}125\\142\end{matrix}\right\}$	$K\beta$	s.	233	$K\alpha$
w.	044	$K\alpha$	w.	115	$K\alpha$	s.	215	$K\alpha$
—	—	—	s.	140	$K\alpha$	w.	216	$K\beta$
—	—	—	w.	141	$K\alpha$	—	—	—
—	—	—	s.	$\left\{\begin{matrix}125\\142\end{matrix}\right\}$	$K\alpha$	—	—	—
—	—	—	w.	135	Ka	—	—	—
—	—	—	w.	136	$K\beta$	—	—	—
—	—	—	w.	126	$K\alpha$	—	—	—

Determined by Westgren and Phragmén from rotating crystal photographs.

$$a:b:c = .891:1:1.329$$

(Groth $a:c = .891:1.329$).

c) Volume

$V = a\cdot b\cdot c = 154.3 \times 10^{-24}\,\mathrm{cm}^3 \qquad d = 7.662$[1])

molecular volume $= 23.43\ \mathrm{cm}^3$

No. of $Fe_3C = 3.99$ in unit of structure.

II. Space Group.

Observed types of absences $(h0l)$ with $(h+l)$ odd

$(0kl)$ with k odd.

Space group V_h^{16}, C_{2v}^9.

---

1) T. Ishigaki, Sci. Rep. Tôhoku, Series I, 16, 295. 1927.

Table II.

Photograph II. Rotation Axis Parallel to the Medium Edge (a_2) of the Elementary Parallelepiped (Westgren and Phragmén).

I	$h_1h_2h_3$	R	I	$h_1h_2h_3$	R	I	$h_1h_2h_3$	R
v. w.	002	$K\alpha$	m.	112	$K\alpha$	v. w.	120	$K\alpha$
w.	200 (?) 103	$K\alpha$ $K\beta$	m.	210	$K\alpha$	m.	120	$K\alpha$
s.	103	$K\alpha$	v. w.	113	$K\beta$	v. w.	121	$K\beta$
v. w.	202 004	$K\beta$	s.	211	$K\alpha$	s.	121	$K\alpha$
m.	202 004	$K\alpha$	s.	113	$K\alpha$	w.	022	$K\beta$
v. w.	105	$K\beta$	m.	212	$K\alpha$	m.	022	$K\alpha$
m.	105	$K\alpha$	m.	114	$K\alpha$	s.	122	$K\alpha$
w.	006	$K\beta$	w.	311	$K\alpha$	v. w.	023	$K\beta$
s.	006	$K\alpha$	m.	312	$K\alpha$	s.	023	$K\alpha$
v. w.	305 (?) 206 403 (?)	$K\beta$	m.	115	$K\alpha$	v. w.	221	$K\alpha$
w.	107	$K\beta$	v. w.	215	$K\beta$	v. w.	123	$K\alpha$
s.	305 (?) 206 403 (?)	$K\alpha$	s.	313	$K\alpha$	w.	222	$K\alpha$
—	—	—	s.	215	$K\alpha$	m.	024	$K\alpha$
—	—	—	s.	314	$K\alpha$	m.	223 124	$K\alpha$
—	—	—	w.	411	$K\alpha$	w.	224 025	$K\beta$
—	—	—	w.	412	$K\alpha$	w.	125	$K\beta$
—	—	—	s.	216 413 (?)	$K\alpha$	s.	224 025	$K\alpha$
—	—	—	—	—	—	s.	125	$K\alpha$

III. Atomic Arrangement.

A center of symmetry is selected as the origin of coordinates.[1]) The possible atomic positions are in general; (V_h^{16})

a) $x\,y\,z;\ \bar{x}, \bar{y}, z+\frac{1}{2};\ \bar{x}+\frac{1}{2}, y+\frac{1}{2}, \bar{z}+\frac{1}{2};\ x+\frac{1}{2}, \bar{y}+\frac{1}{2}, \bar{z}$

$\bar{x}\,\bar{y}\,\bar{z};\ x, y, \bar{z}+\frac{1}{2};\ x+\frac{1}{2}, \bar{y}+\frac{1}{2}, z+\frac{1}{2};\ \bar{x}+\frac{1}{2}, y+\frac{1}{2}, z$

with two degrees of freedom, on the reflection planes;

b) $u\,v\,\frac{1}{4};\ \bar{u}\,\bar{v}\,\frac{3}{4};\ \bar{u}+\frac{1}{2}, v+\frac{1}{2}, \frac{1}{4};\ u+\frac{1}{2}, \bar{v}+\frac{1}{2}, \frac{3}{4}$

without degrees of freedom, at the centers of symmetry;

c) $0\,0\,0;\ 0\,0\,\frac{1}{2};\ \frac{1}{2}\,\frac{1}{2}\,0;\ \frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$

d) $\frac{1}{2}\,0\,0;\ \frac{1}{2}\,0\,\frac{1}{2};\ 0\,\frac{1}{2}\,0;\ 0\,\frac{1}{2}\frac{1}{2}$.

---

1) P. Niggli, Geometrische Kristallographie des Diskontinuums, 201, Leipzig 1919.

Table III.

Photograph III. Rotation Axis Parallel to the Longest Edge (a_3) of the Elementary Parallelepiped. (Westgren and Phragmén.)

I	$h_1h_2h_3$	R	I	$h_1h_2h_3$	R	I	$h_1h_2h_3$	R	I	$h_1h_2h_3$	R
w.	200(?) 210	$K\alpha$ $K\beta$	w.	021	$K\alpha$	m.	112	$K\alpha$	m.	103	$K\beta$
w.	120	$K\alpha$	v. w.	121	$K\beta$	v. w.	022	$K\beta$	s.	113	$K\alpha$
s.	210	$K\alpha$	v. w.	211	$K\beta$	s.	022	$K\alpha$	m.	023	$K\alpha$
w.	130	$K\alpha$	s.	121	$K\alpha$	v. w.	202 122	$K\beta$	w.	223	$K\alpha$
v. w.	140	$K\beta$	s.	211	$K\alpha$	s.	202 122	$K\alpha$	w.	313	$K\beta$
v. w.	330	$K\beta$	w.	221	$K\alpha$	w.	212	$K\alpha$	w.	233	$K\beta$
s.	140	$K\alpha$	w.	131	$K\alpha$	w.	222	$K\alpha$	s.	313	$K\alpha$
s.	330	$K\alpha$	w.	311	$K\alpha$	v. w.	312	$K\beta$	s.	233	$K\alpha$
s.	240	$K\alpha$	w.	141	$K\alpha$	s.	312	$K\alpha$	—	—	—
w.	150 500(?)	$K\beta$	m.	331	$K\alpha$	w.	232	$K\alpha$	—	—	—
—	—	—	m.	411	$K\alpha$	v. w.	042	$K\alpha$	—	—	—
—	—	—	m.	421	$K\alpha$	v. w.	142	$K\alpha$	—	—	—
—	—	—	—	—	—	w.	332	$K\alpha$	—	—	—
—	—	—	—	—	—	w.	242	$K\alpha$	—	—	—

The following five possible arrangements of iron atoms are to be considered:

I. $8\,Fe$ at (a), $4\,Fe$ at (b)
II. $8\,Fe$ at (a), $4\,Fe$ at (c)
III. $8\,Fe$ at (a), $4\,Fe$ at (d)
IV. $4\,Fe$ at (b), $4\,Fe$ at (c), $4\,Fe$ at (d)
V. $4\,Fe$ at (b), $4\,Fe$ at (b), $4\,Fe$ at (b).

The observed intensities of reflection of (001) in different orders, see Table I, cannot be explained by arrangements II, III, IV, and V if the iron atoms at $x\,y\,z$ and at $x, y, \bar{z}+\frac{1}{2}$, etc., are to be at least 1.5 Å apart.

IV. Evaluation of the Parameters.

The positions of the iron atoms are defined by five parameters. Since these parameters are separable, it is possible to determine rigorously their values. The structure factors for (hkl) reduce to the following four cases:

$$(o\,o\,o);\ (e\,e\,o);\ [(e) = \text{even}\ (o) = \text{odd}]$$

$$\frac{A}{4\,F_{Fe}} = 2\cos 2\pi(hx)\sin 2\pi(ky)\sin 2\pi(lz) + \cos 2\pi(hu)\sin 2\pi(kv)\sin 2\pi(l/4)$$

$$B = 0$$

$(e\,e\,e);\ (o\,o\,e)$

$$\frac{A}{4\,F_{Fe}} = 2\cos 2\pi(hx)\cos 2\pi(ky)\cos 2\pi(lz) + \cos 2\pi(hu)\cos 2\pi(kv)\cos 2\pi(l/4)$$

$$B = 0$$

$(e\,o\,o);\ (o\,e\,o)$

$$\frac{A}{4\,F_{Fe}} = 2\sin 2\pi(hx)\cos 2\pi(ky)\sin 2\pi(lz) + \sin 2\pi(hu)\cos 2\pi(kv)\sin 2\pi(l/4)$$

$$B = 0$$

$(e\,o\,e);\ (o\,e\,e)$

$$\frac{A}{4\,F_{Fe}} = 2\sin 2\pi(hx)\sin 2\pi(ky)\cos 2\pi(lz) + \sin 2\pi(hu)\sin 2\pi(kv)\cos 2\pi(l/4)$$

$$B = 0.$$

One must consider all values of x and u from .00 to 1.00; y and v from .00 to .50 and z from .00 to .25; except in so far as combinations of x, y, u and v are limited by symmetry requirements.

a) The observed orders of intensities, (002) v. w., (004) with (023) or with (202)m, and (006)v. s., can only be explained by a value of z near .06 — .07. The value is taken to be .65 ± .015.

b) Planes of the type $(0kl)$ can be used for the determination of v and y in conjunction with $z = .065 \pm .015$. The following intensity relationships require:

$$v = .05 \pm .02 \quad \text{or} \quad v = .20 \pm .02$$
$$y = .17 \pm .02 \qquad\quad y = .09 \pm .02$$

(1) (025) st $>$ (023)m (requires $\sin 2\pi(2y)$ to have the same sign as $\sin 2\pi(2v)$)

(2) (022) st $>$ (020)a

(3) The absence of reflections from (020) and (024)

(4) The observed orders of intensity

(041)a, (043)st, (040)a, (042)v. w.

c) Planes of the type $(h0l)$ can be used for the determination of u and x in conjunction with $z = .065 \pm .015$. The following intensity relationships require:

$$x = \ \ .17 \pm .02 \quad \text{or} \quad x = \ \ .34 \pm .02$$
$$u = -.16 \pm .03 \qquad\quad u = -.16 \pm .03$$

(1) (103) st > (105) m; (101) a (requires $\sin 2\pi(x)$ to be opposite in sign to $\sin 2\pi(u)$)
(2) (105) m > (101) a; (105) required to have medium intensity
(3) (105) m > (303) a
(4) (103) st > (301) a; and (105) m > (301) a
(5) (101) and (301) required to be absent or very weak.

d) Planes of the type ($hk0$) can be used for elimination of some of the possible combinations of values of x and u with those of v and y; there are four permutations. The following eliminations are effected:

(1) (210) st > (110) a

$$x = .17 \pm .02$$
$$u = -.16 \pm .03.$$

(2) The observed absence or very low intensity of reflections from (230), (310) and (110) eliminates

$$v = .20 \pm .02$$
$$y = .09 \pm .02.$$

Accuracy of the Derived Structure.

The parameter values derived from considerations of intensities of reflections from ($hk0$), ($0kl$) and ($h0l$) are

$$z = .065 \pm .015 \qquad y = .17 \pm .02 \qquad u = -.16 \pm .03.$$
$$v = .05 \pm .02 \qquad x = .34 \pm .02$$

Data from planes of the type (hkl) can now be used to check this structure. The concomitance of observed intensities and calculated structure factors is shown for a number of planes in Table IV. There can be but little doubt that the parameter values are accurate to within the given limits.

Geometrical Characteristics of the Derived Structure.

The unit of structure containing $4Fe_3C$ is shown as Figure 1. From this figure, and Figure 2, it is apparent that each iron atom is at the corner of two octahedra; one such octahedron is formed by (1) (2) (3) (4) (5) and (6) of Figure 1. In general it is possible for this octahedron to be a regular one but within the listed limitation of the parameters it must be a distorted one; in particular it must be distorted to prevent too close approach of atoms such as (2) and (7). Using the determined parameter values one finds that the sides of the octahedron have the lengths: 2.68, 2.56, 2.56, 2.56, 2.55, 2.57, 2.66, 2.73, 2.73, 2.66, 2.57, and 2.55 Å. These values are of no exact significance since they

Table IV.

Calculated Structure Factors for Various Planes of Cementite.

Plane	Intensity	d_{hkl}	$A^2/16F^2_{Fe}$	Plane	Intensity	d_{hkl}	$A^2/16F^2_{Fe}$
101		3.752	0.03	222	w.	1.51	0.45
002	v. w.	3.369	(0.14)[1]	024	m.	1.40	(0.77)
200	w.	2.26	(1.66)	223		1.35	0.47
103	s.	2.01	5.85	124	m.	1.34	0.35
202		1.88	0.02	320		1.29	(0.07)
004	m.	1.68	(0.77)	321		1.27	0.02
301		1.47	0.00	322		1.21	0.05
204		1.35	0.14	025	s.	1.19	(4.37)
105	m.	1.29	0.42	224		1.19	0.14
303		1.25	0.12	125	s.	1.15	2.28
400	s.	1.13	(3.69)				
006	s.	1.12	(6.45)	110		3.37	0.00
402		1.07	0.06	020		2.53	(0.07)
305		1.00	0.01	200	w.	2.26	1.66
206	s.	1.00	1.19	120	w.	2.21	0.86
				210	s.	2.06	3.54
110		3.37	(0.01)	220		1.69	0.01
111		3.02	0.04	130	w.	1.58	1.71
112	m.	2.38	0.74	310		1.44	0.00
210	m.	2.06	(3.84)	230		1.35	0.39
211	s.	1.97	1.44	320		1.29	0.01
113	s.	1.87	1.10	040		1.27	(0.30)
212	m.	1.76	0.67	140	s.	1.20	5.52
213		1.52	0.00	400		1.13	(3.68)
114	m.	1.51	0.32	330	s.	1.12	6.60
310		1.44	(0.00)	240		1.10	0.06
311	w.	1.41	0.14	410	s.	1.10	1.25
312	m.	1.33	2.53	420		1.03	0.04
214		1.30	0.03	150	w.	.989	0.76
115	m.	1.25	0.34	340		.970	0.11
313	s.	1.21	3.65	430		.939	0.27
215	s.	1.13	2.69				
410	s.	1.10	(2.53)	101		3.75	(0.03)
314 ?		1.09	1.00	111		3.02	0.04
411 ?	w.	1.09	1.04	021	m.	2.37	(1.54)
116		1.06	0.01	121	s.	2.10	1.21
412	w.	1.05	0.49	211	s.	1.97	1.44
413		.990	0.00	221	w.	1.64	0.62
315		.986	1.51	131	w.	1.54	0.21
216	s.	.987	2.28	301		1.47	(0.00)

---

[1] Complete rotation corresponds to reflection from only two members of the form for all structure factors given in parenthesis.

Table IV (Continued).

Plane	Intensity	d_{hkl}	$A^2/16F^2_{Fe}$	Plane	Intensity	d_{hkl}	$A^2/16F^2_{Fe}$
311	w.	1.41	0.14	132		1.45	0.17
231		1.33	0.02	312	s.	1.33	2.53
321		1.27	0.02	232	w.	1.26	0.66
041		1.24	(0.05)	322		1.21	0.05
141	w.	1.20	0.29	042	v. w.	1.19	(0.08)
331	m.	1.11	0.72	142	v. w.	1.15	0.06
241		1.09	0.01	332	w.	1.07	0.59
411	m.	1.09	1.04	242	w.	1.05	0.16
421	m.	1.02	0.66				
				103	s.	2.01	(5.85)
112	m.	2.38	0.74	113	s.	1.87	1.10
022	s.	2.03	(2.43)	023	m.	1.68	(0.90)
202		1.88	(0.02)	123		1.57	0.02
122	s.	1.85	2.22	213		1.52	0.00
212	w.	1.76	0.67	223	w.	1.35	0.17
222	w.	1.51	0.45				

are affected by changes of parameter values, but they cannot all be equal.

Inspection of space models and analytical examination shows that each of the iron atoms in the reflection plane is approximately equidistant from twelve other iron atoms. The distances are: 2.73, 2.66, 2.57, 2.55, 2.55, 2.57, 2.73, 2.66. 2.68, 2.68, 2.66, and 2.66 Å. Each of the iron atoms in the general positions is about equidistant from eleven other iron atoms. The distance are: 2.68, 2.57, 2.56, 2.73, 2.56, 2.66, 2.55, 2.68, 2.43, 2.66, and 2.43 Å. In these instances, as for the case given in the preceding paragraph, the particular values are not to be emphasized since variation of the parameter values within the limits determined would cause shifts in these distances that could be as great as .2 Å. In no case, however, are all the values equal.

The structure can best be described as a coordination one composed of octahedra of iron atoms that are joined by the sharing of corners. Each octahedron shares each of its corners with one other octahedron. These second octahedra do not share corners with second octahedra; four octahedra are required to form a closed figure. These relationships can perhaps more clearly be seen in Fig. 2 and 3. The space model Fig. 3 also shows that the edges of the octahedra are not all related in the same manner to the adjacent octahedra; a fact that is probably connected with the distance variations listed above.

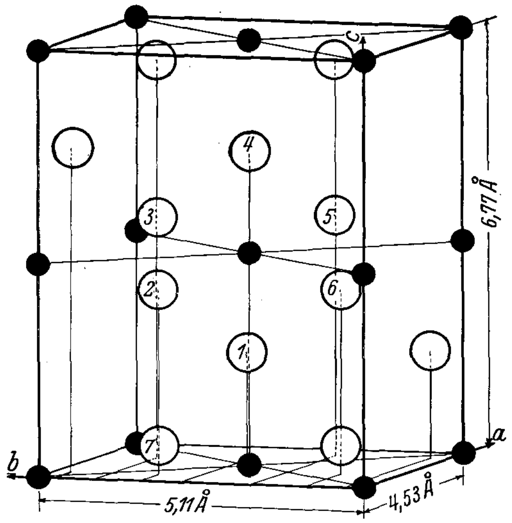

Fig. 1. A representation of the unit of structure containing $4\,Fe_3C$.

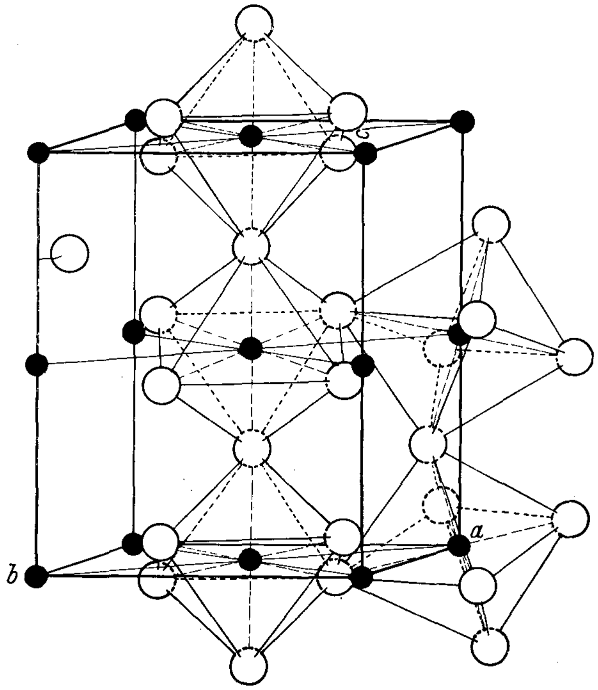

Fig. 2. A drawing showing the structure of Fe_3C as built from octahedra of iron atoms around central carbon atoms.

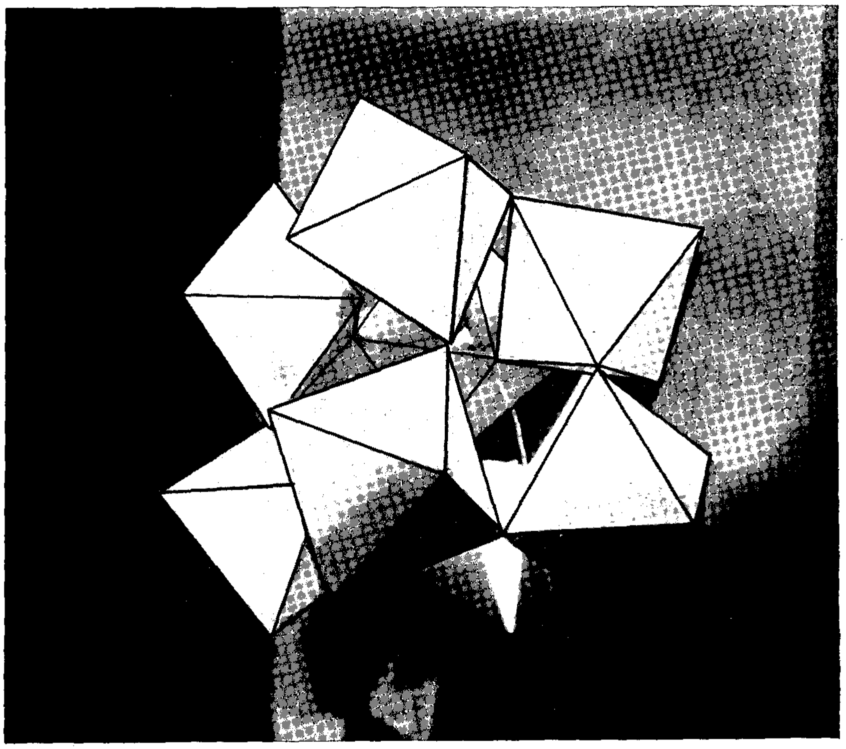

Fig. 3. An array of octahedra of iron atoms partially illustrating the structure of cementite.

Positions of the Carbon Atoms.

It has been possible to account for all observed intensities of reflections without considering the positions of the carbon atoms. It might be thought that the carbon atoms could be in positions other than those required by V_h^{16}. A comparison of the F curves for carbon and iron, however, shows that the carbon must have some detectable effect upon the intensities of reflection. Planes of the type $(h0l)$ with $(h+l)$ odd and $(0kl)$ with k odd are strictly absent, in particular (010), (001) and (100) that I have tried to detect on over exposed oscillating crystal photographs. It would seen then that the carbon atoms too require the space group V_h^{16}, although the evidence it not conclusive.

Four carbon atoms can be located at either of the two sets of symmetry centers or on the planes of symmetry. One can differentiate between these possibilities only on the basis of probable geometrical configuration. If the carbon atoms were on planes of symmetry the resulting structure would be a most unusual one. The symmetry centers, 000, $00\frac{1}{2}$, $\frac{1}{2}\frac{1}{2}0$, and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, however, are the centers of the coordination octahedra of iron atoms. It would seem to be most logical that the carbon atoms should be in these positions. If this is true the *Fe—C* distances are ca. 1.82, 1.86, and 1.89 Å.

Discussion.

From the preceding descriptions one sees that cementite can be considered as a coordination structure of octahedra of iron atoms around central carbon atoms. This interpretation suggests that the general rules formulated by Pauling¹) in his coordination theory of the structure of ionic compounds, can in part be extended to crystals that are not ionic. The case of Fe_3C alone does not suffice to indicate the way in which Pauling rules must be modified for these particular kinds of compounds. The more strictly geometrical rules III and V seem to be capable of general application. They are adhered to by cementite.

V. M. Goldschmidt²) and L. Pauling³) have derived atomic and ionic radii for various elements. They give the radius of Fe^{++} as .75 Å. In cementite it is to be noted that the *Fe—Fe* distances are approximately those of metallic iron (2.54 Å for a coordination number of 12). It would thus seem that cementite is composed of iron atoms, similar to those of metallic iron, with $r_{Fe} =$ ca. 1.3 Å. The carbon to iron distances are 1.82 Å, 1.86 Å, and 1.89 Å. These distances with the above value of r_{Fe} require $r_C =$ ca. 55 Å. It seems to be quite improbable that the carbon atom could have a negative charge. The structure is probably not ionic in type.

Finally one might comment that the observed absence of the formation of solid solutions in the iron carbon system between cementite and phases containing more or less carbon than it contains can adequately be explained by the derived structure. The structure can also account for the hardness of Fe_3C and for the lack of metallographic characteristics that would require similarity of arrangement of iron atoms in some plane of cementite compared with a specific plane of α iron.

I am particularly indebted to Prof. Westgren for the courtesy that he has shown. Dr. P. R. Kosting and Mr. M. E. Jefferson assisted in the structure determination.

---

1) L. Pauling, J. Am. chem. Soc. **51**, 1016. 1929.

2) V. M. Goldschmidt, Trans. Faraday Soc. **25**, 260. 1929.

3) Linus Pauling, J. Am. chem. Soc. **49**, 765. 1927.

Summary.

The crystal structure of cementite has been derived from the x-ray diffraction data of Westgren and Phragmén. The orthorhombic unit of structure containing $4\,Fe_3C$ has the dimensions $a = 4.518$ Å, $b = 5.069$ Å, $c = 6.736$ Å. (Westgren and Phragmén.) The space group is V_h^{16}; the atomic positions are:

$8\,Fe$ at (a) $x\,y\,z;\; \bar{x}\bar{y},\, z+\frac{1}{2};\; \bar{x}+\frac{1}{2},\, y+\frac{1}{2},\, \bar{z}+\frac{1}{2};\; x+\frac{1}{2},\, \bar{y}+\frac{1}{2},\, \bar{z}$
$\bar{x}\,\bar{y}\,\bar{z};\; xy,\, \bar{z}+\frac{1}{2};\; x+\frac{1}{2},\, \bar{y}+\frac{1}{2},\, z+\frac{1}{2};\; \bar{x}+\frac{1}{2},\, y+\frac{1}{2},\, z$
$4\,Fe$ at (b) $u\,v\,\frac{1}{4};\; \bar{u}\bar{v}\frac{3}{4};\; \bar{u}+\frac{1}{2},\, v+\frac{1}{2},\, \frac{1}{4};\; u+\frac{1}{2},\, \bar{v}+\frac{1}{2},\, \frac{3}{4}$
$4\,C$ at (c) $000;\; 00\frac{1}{2};\; \frac{1}{2}\frac{1}{2}0;\; \frac{1}{2}\frac{1}{2}\frac{1}{2}$.

The parameter values are:

$x = .34 \pm .02;\; y = .17 \pm .02;\; z = .065 \pm .015;\; v = .05 \pm .02;$
$u = -.16 \pm .03.$

The structure is an excellent illustration of a coordination type structure.

Bureau of Chemistry and Soils,
U. S. Departement of Agriculture, Washington, D. C.

Received April 28th, 1930.