

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  $\frac{1}{2}$ , are more stable than non-resonating bonds, with bond number 1. The actual FeSi structure would thus be preferred to the cesium

\* 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).

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

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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 *Umklaupung* 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.

A definite orientation relation exists between the original and final structures in any phase change which occurs by a crystallographic deformation process. For the transformation from austenite to martensite the orientation relation has been experimentally established by Kurdjumow & Sachs (1930) and by Wasserman (1935). A  $\{111\}$  plane of austenite is parallel to a  $\{110\}$  plane of martensite, and, in these two parallel planes, a  $\langle 110 \rangle$  direction of austenite is parallel to a  $\langle 111 \rangle$  direction of martensite; the indices are referred to the usual orthogonal axes for face-centred cubic and body-centred cubic structures respectively. This lattice relationship admits of twenty-four crystallographically equivalent variants; in this paper only one of these is explicitly treated, but it can be shown that equivalent results would be obtained if any other of the possible orientation relations were selected. In practice only one orientation relation is found in a single transformation unit, but all of the possible variants may occur in different transformation units within the same bulk specimen.

The form of the region within an austenite grain to which a single *Umklappung* process will extend is, in general, plate-like, so that the transformation units are seen as needle-shaped traces in any arbitrary section chosen for microscopic examination after the phase change is complete. The trace of the habit plane itself appears as a prominent central straight line in the martensite needle, as is illustrated in Fig. 1; this is generally referred to as a midrib. By observation of this trace of the habit plane for a single martensite plate in two or more different plane sections the crystallographic orientation of the habit plane can be determined. Greninger & Troiano (1940) have found that the plane can be described as  $\{259\}_\gamma$  for steels containing more than 1.4% carbon, and as  $\{225\}_\gamma$  for steels containing from 0.55 to 1.4% carbon. (The suffix  $\gamma$  refers to the fact that the indices are given relative to the reference axes used for the austenite or  $\gamma$  structure; the suffix  $\alpha$  will similarly be used for indices referred to the martensite axes.) In steels containing less than about 0.55% carbon martensite transformation units are needle-shaped rather than plate-like, but as the needles themselves tend to group in plate-like arrays which delineate  $\{111\}_\gamma$  planes, this can be considered as defining a habit plane of martensite for these low-carbon steels.

Many attempts have been made to develop a simple pictorial description of the mechanism of the transformation from austenite to martensite. Bain (1924) first pointed out that, as illustrated in Fig. 2, a face-centred cubic structure can be alternatively considered as being built up from body-centred tetragonal units, and therefore that three mutually orthogonal simple strains could transform it to a body-centred cubic or body-centred tetragonal structure of any required structure cell size. Kurdjumow & Sachs proposed a mechanism for the transformation from

austenite to martensite which was designed to account for the orientation relation which they had observed between the two structures; this consisted of a shear of one of the  $\{111\}$  austenite planes by  $19^\circ 28'$ , followed by a second smaller shear within that plane, and finally by minor dimensional adjustments. This mechanism accounted satisfactorily for the orientation of the martensite relative to the parent austenite, but not for the observed irrational habit plane of martensite plates. Greninger & Troiano, as a result of measurements of the relief effects produced on free surfaces in austenite by the transformation of single martensite plates, proposed a transformation mechanism in which a homogeneous shear occurred on the plane of the martensite plate, a second smaller shear followed which was not homogeneous but occurred stepwise in units much smaller than that of the martensite plate, and final dimensional adjustments completed the structural change.

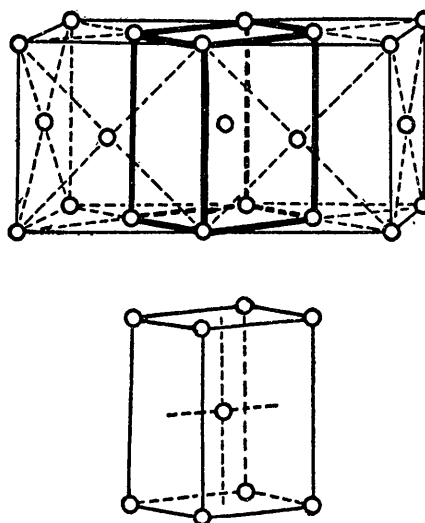


Fig. 2. Body-centred tetragonal lattice delineated in austenite (face-centred cubic) structure. (After Bain (1924).)

In effect, all postulated transformation mechanisms of this kind arbitrarily prescribe paths for the atoms in moving from their initial to their final positions. The actual paths must be very much more complex than the simple straight-line sequences which have been suggested, since they are determined by considerations of the potential-energy functions between the two sets of positions. Furthermore, we have no experimental evidence about the paths, but are only able to observe the original and final positions of the atoms. In the present treatment, therefore, no consideration is given to the atomic paths, but a unique correspondence is set up between the positions of the atoms in the austenite and martensite structures. This is done by determining the relative orientation of the two phases from the experimentally observed lattice relationships, and by making use of the assumption that of all the possible



Fig. 1. Martensite and austenite in 1.78% carbon steel.  $\times 1000$ .  
(After Greninger & Troiano (1940).)

distortions of a primitive unit cell of the face-centred cubic structure, which could generate a body-centred cubic structure of the given relative orientation, the one which actually occurs is the smallest. This purely mathematical treatment is an approach to the martensite transformation which is at once more general and more powerful than any of the necessarily arbitrary crystallographic descriptions.

## 2. Discussion of mathematical methods

The discussion of the atomic displacements in the transformation from austenite to martensite will be largely concerned with the relationship between various rectangular axis-systems, because to establish a unique correspondence between individual atomic sites in the two structures we must be able to talk about both sets of atomic positions with reference to a common system of reference axes, and at the moment we know the arrangement of atomic co-ordinates in both structures only relative to the ordinary crystallographic axes to which they are normally referred. We must therefore develop a method for translating atomic co-ordinates known relative to one of the axis-systems into terms of the other axis-system, or, alternatively, we could translate both into terms of a third independent system of axes of reference.

For the treatment of relationships between different systems of axes of reference, the symbolism and properties of matrices offer a natural means of expression. Thus consider two rectangular axis-systems  $P$  and  $Q$ . If a point had co-ordinates

$$(x_p, y_p, z_p) \text{ in } P \quad \text{and} \quad (x_q, y_q, z_q) \text{ in } Q,$$

then, by the well-known formulae for transformation of axes,

$$\left. \begin{aligned} x_q &= l_1 x_p + m_1 y_p + n_1 z_p, \\ y_q &= l_2 x_p + m_2 y_p + n_2 z_p, \\ z_q &= l_3 x_p + m_3 y_p + n_3 z_p, \end{aligned} \right\} \quad (1)$$

where  $l_1$  is the cosine of the angle between  $OX_q$  and  $OX_p$ ,  $m_1$  is the cosine of the angle between  $OX_q$  and  $OY_p$ , and similarly for the other terms.

In these equations the array of cosine terms will be the same for all points such as  $(x_p, y_p, z_p)$ , and is, in fact, the characteristic invariant feature of the axis transformation itself. It is therefore convenient to separate it from the variables, i.e. the co-ordinates such as  $x_p, y_p$ , etc., and to represent (1) in the purely symbolic form

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}_q = \begin{pmatrix} l_1 & m_1 & n_1 \\ l_2 & m_2 & n_2 \\ l_3 & m_3 & n_3 \end{pmatrix} \times \begin{pmatrix} x \\ y \\ z \end{pmatrix}_p. \quad (1a)$$

The array of cosine terms in the second bracket of equation (1a), which is called the matrix of the axis transformation from axes  $P$  to axes  $Q$ , completely defines the relative orientation of the axes  $Q$  to  $P$ .

Following Dirac, an array of this type may be abbreviated to  $(Q/P)$ .

The convenience of the matrix notation is that there are simple rules for the independent mathematical treatment of matrices. For example, if  $R$  is a third axis-system, whose orientation is known relative to  $Q$ , i.e. we know that

$$(R/Q) = \begin{pmatrix} L_1 & M_1 & N_1 \\ L_2 & M_2 & N_2 \\ L_3 & M_3 & N_3 \end{pmatrix},$$

then the matrix of the transformation from axes  $P$  to axes  $R$  is given as the matrix product of the two intermediate axis transformations, i.e.

$$\begin{aligned} (R/P) &= (R/Q) \times (Q/P) \\ &= \begin{pmatrix} L_1 & M_1 & N_1 \\ L_2 & M_2 & N_2 \\ L_3 & M_3 & N_3 \end{pmatrix} \times \begin{pmatrix} l_1 & m_1 & n_1 \\ l_2 & m_2 & n_2 \\ l_3 & m_3 & n_3 \end{pmatrix} \\ &= \begin{pmatrix} L_1 l_1 + M_1 l_2 + N_1 l_3 & L_1 m_1 + M_1 m_2 + N_1 m_3 & L_1 n_1 + M_1 n_2 + N_1 n_3 \\ L_2 l_1 + M_2 l_2 + N_2 l_3 & L_2 m_1 + M_2 m_2 + N_2 m_3 & L_2 n_1 + M_2 n_2 + N_2 n_3 \\ L_3 l_1 + M_3 l_2 + N_3 l_3 & L_3 m_1 + M_3 m_2 + N_3 m_3 & L_3 n_1 + M_3 n_2 + N_3 n_3 \end{pmatrix}. \end{aligned}$$

The use of matrices is not confined to axis transformations. Matrices of all types of linear transformations have similar properties and are extensively used in the text.

## 3. Relative orientation of austenite and martensite

The validity of the Kurdjumow-Sachs lattice relationship is a prime assumption of the present treatment of the transformation from austenite to martensite. For detailed discussion we shall select a single one of the twenty-four possible variants of this relationship, the particular one chosen being

$$(111)_\gamma \parallel (101)_\alpha, \quad [\bar{1}\bar{1}0]_\gamma \parallel [11\bar{1}]_\alpha. \quad (3)$$

As mentioned earlier, we shall assume in the first instance that we are dealing with a hypothetical martensite-type reaction between the  $\gamma$  and  $\alpha$  forms of pure iron, and so we can for the moment neglect the tetragonality of martensite and assume that in both structures directions are normal to planes of the same indices. We can then express relation (3) alternatively by the parallelism of the three pairs of directions

$$\left. \begin{aligned} (a) \quad & [111]_\gamma \parallel [101]_\alpha \dots\dots I_z, \\ (b) \quad & [\bar{1}\bar{1}0]_\gamma \parallel [11\bar{1}]_\alpha \dots\dots I_y, \\ (c) \quad & [\bar{1}\bar{1}2]_\gamma \parallel [1\bar{2}\bar{1}]_\alpha \dots\dots I_x. \end{aligned} \right\} \quad (4)$$

Relation (a) holds because the two directions mentioned are normal to planes which are themselves parallel, relation (b) comes directly from the lattice relationship

in equation (3), and relation (c) follows because  $I_x$  is perpendicular to both  $I_y$  and  $I_z$  and must therefore be uniquely defined in direction.

The three directions  $I_x, I_y, I_z$  form a convenient intermediate rectangular frame of reference  $I$ , the relations of which to the usual austenite cube axes  $A$ , and the martensite cube axes  $M$ , are known from the

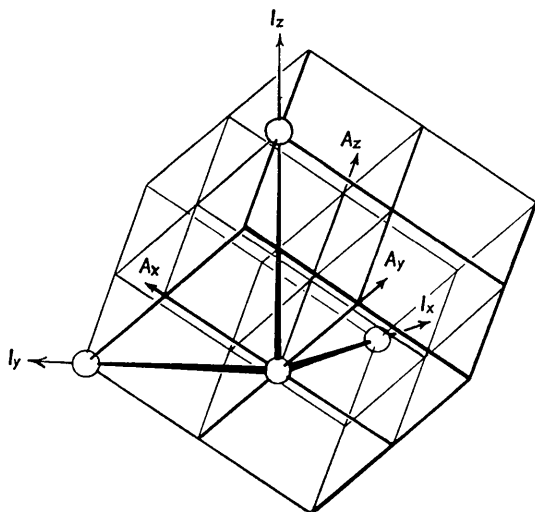


Fig. 3. Relation between the austenite cube axes  $A$  and the lattice-relationship axes  $I$ .

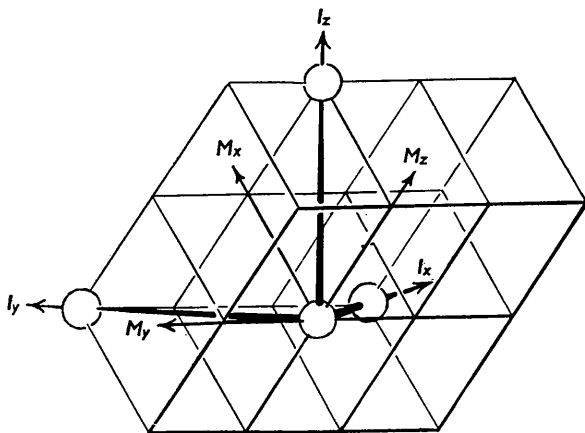


Fig. 4. Relation between the martensite cube axes  $M$  and the lattice-relationship axes  $I$ .

indices specified on the left- and right-hand sides respectively of relation (4). The relation between axes  $I$  and axes  $A$  is illustrated in Fig. 3, and that between axes  $I$  and axes  $M$  in Fig. 4. From the indices of the  $I$  axes relative to the  $A$  and  $M$  axes the corresponding direction cosines may be directly evaluated, and so the axis-transformation matrices from axes  $A$  to axes  $I$  and from axes  $M$  to axes  $I$  can be determined. From these two matrices the matrix of the axis transformation from axes  $A$  to axes  $M$  is then obtained by matrix multiplication:

$$(M/A) = (M/I) \cdot (I/A)$$

$$= \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & \sqrt{2} & \sqrt{3} \\ \bar{2} & \sqrt{2} & 0 \\ \bar{1} & \sqrt{2} & \sqrt{3} \end{pmatrix} \cdot \frac{1}{\sqrt{6}} \begin{pmatrix} \bar{1} & \bar{1} & 2 \\ \sqrt{3} & \sqrt{3} & 0 \\ \sqrt{2} & \sqrt{2} & \sqrt{2} \end{pmatrix},$$

$$\text{i.e. } (M/A) = \frac{1}{6} \begin{pmatrix} \bar{1} + 2\sqrt{6} & \bar{1} & 2 + \sqrt{6} \\ 2 + \sqrt{6} & 2 + \sqrt{6} & \bar{4} \\ 1 & 1 + 2\sqrt{6} & \bar{2} + \sqrt{6} \end{pmatrix}. \quad (5)$$

In (5) we have established in mathematical form a direct relation between the  $A$  and  $M$  axis-systems such that, given the co-ordinates of a point relative to either of them, we can determine its co-ordinates relative to the other axis-system. At this stage we may profitably

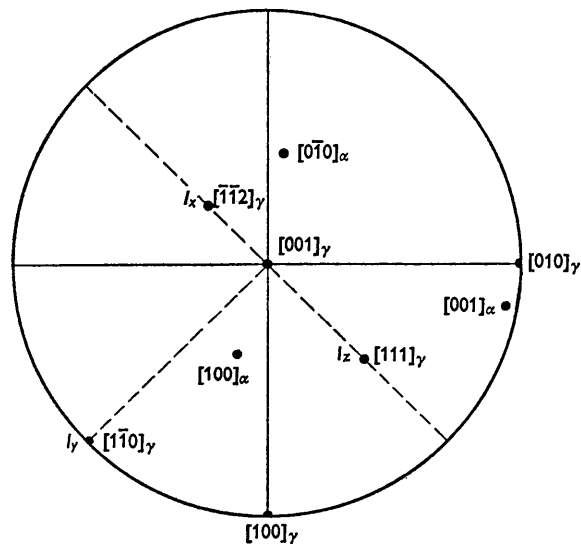


Fig. 5. Stereogram illustrating the relative orientation of the austenite ( $\gamma$ ) cube axes, the martensite ( $\alpha$ ) cube axes, and the lattice-relationship axes.

state the assumptions which have been made in establishing this relation; these are:

- (1) The orientation relation between the original and final structures is that specified in (3).
- (2) The origins of co-ordinates for the axis-systems  $A$  and  $M$  are coincident.

Using these same assumptions, the same relation as is given in equation (5) can be developed stereographically; a stereogram showing the relation of both axes  $I$  and axes  $M$  to axes  $A$  is given in Fig. 5. For the purposes of the present paper, however, the mathematical expression of the axis relation given in equation (5) is the more useful one.

We now wish to use equation (5) to refer to axes  $M$  the co-ordinates of an atomic site known relative to axes  $A$ . Consider, for example, the atomic site

$$(xa, ya, za)_A,$$

where  $x, y, z$  are co-ordinate numbers,  $a$  the lattice parameter of austenite for zero carbon content

( $a=3.564$  A.), and the subscript  $A$  indicates the system of reference. If the co-ordinates of this same atomic site relative to axes  $M$  are  $(x\alpha, y\alpha, z\alpha)_M$ , where  $x, y, z$  are co-ordinate numbers,  $\alpha$  is the lattice parameter of martensite extrapolated to zero carbon content ( $\alpha=2.860$  A.) and the subscript  $M$  refers to the axis-system, then the following relation holds:

$$\begin{pmatrix} x\alpha \\ y\alpha \\ z\alpha \end{pmatrix}_M = (M/A) \cdot \begin{pmatrix} x\alpha \\ y\alpha \\ z\alpha \end{pmatrix}_A \quad (6)$$

The relation expressed in (6) is one between co-ordinates; it will be more convenient to rewrite this so as to express the relation between co-ordinate numbers. We obtain

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}_M = \frac{a}{\alpha} \cdot (M/A) \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix}_A \quad (7)$$

and the matrix  $\frac{a}{\alpha} (M/A)$  is evaluated as

$$\begin{pmatrix} 0.810 & \overline{0.208} & 0.924 \\ 0.924 & \overline{0.093} & \overline{0.831} \\ 0.208 & 1.225 & 0.093 \end{pmatrix}.$$

Using this matrix, we can, by equation (7), refer to axes  $M$  the co-ordinate numbers of any atomic site whose co-ordinate numbers are known relative to axes  $A$ .

#### 4. Atomic displacements

The co-ordinates of an atom in austenite, relative to axes  $A$ , are of the form  $(\frac{1}{2}n_1a, \frac{1}{2}n_2a, \frac{1}{2}n_3a)_A$ , where  $n_1, n_2, n_3$  are integers. Because the structure is face-centred cubic the integers must satisfy the condition that  $n_1+n_2+n_3$  is even. In martensite, atomic co-ordinates referred to axes  $M$  are of the form

$$(\frac{1}{2}\nu_1\alpha, \frac{1}{2}\nu_2\alpha, \frac{1}{2}\nu_3\alpha)_M,$$

where  $\nu_1, \nu_2, \nu_3$  are integers, and, because the structure is body-centred cubic, the three integers must all be like, i.e. either all even or all odd.

We now wish to consider the atomic displacements involved in generating the martensite structure from austenite, and we assume that these must constitute a homogeneous deformation of the entire structure. Such a homogeneous deformation is completely defined if we determine the displacements of the atoms constituting a primitive unit cell in austenite. We select for consideration the primitive cell effectively defined by the four atoms whose co-ordinate numbers are

$$(0, 0, 0)_A, \quad (\frac{1}{2}, \frac{1}{2}, 0)_A, \quad (\frac{1}{2}, 0, \frac{1}{2})_A, \quad (0, \frac{1}{2}, \frac{1}{2})_A.$$

By using the relation expressed in (7) we can determine the co-ordinate numbers of these four atoms

relative to the martensite axes of reference. These are as follows:

$$\left. \begin{aligned} (0, 0, 0)_A &\equiv (0, 0, 0)_M, \\ (\frac{1}{2}, \frac{1}{2}, 0)_A &\equiv (0.301, 0.416, 0.717)_M, \\ (\frac{1}{2}, 0, \frac{1}{2})_A &\equiv (0.867, 0.047, 0.151)_M, \\ (0, \frac{1}{2}, \frac{1}{2})_A &\equiv (0.358, \overline{0.462}, 0.659)_M. \end{aligned} \right\} \quad (8)$$

It should be emphasized that (8) expresses only a transformation to the  $M$  reference axes, and that we have not yet considered any displacements of the atoms.

We know that when the transformation to martensite occurs the co-ordinate numbers relative to axes  $M$  of the four atoms under consideration must change from those given on the right-hand side of (8) to co-ordinate numbers of the type  $(\frac{1}{2}\nu_1, \frac{1}{2}\nu_2, \frac{1}{2}\nu_3)$ , where  $\nu_1, \nu_2, \nu_3$  are like integers. We have to identify the particular sites of this type to which the atoms in question move. We shall assume that, of the many possible distortions of a primitive unit cell of austenite by which the martensite structure could be generated, the one which actually occurs is the smallest. This is equivalent to stating that the four atoms which we are considering will move on transformation from the positions indicated on the right-hand side of (8) to the nearest available atomic sites on the martensite lattice. We can therefore immediately identify the displacements of the four atoms in question as being

$$\left. \begin{aligned} (0, 0, 0)_M &\rightarrow (0, 0, 0)_M, \\ (0.301, 0.416, 0.717)_M &\rightarrow (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})_M, \\ (0.867, 0.047, 0.151)_M &\rightarrow (1, 0, 0)_M, \\ (0.358, \overline{0.462}, 0.659)_M &\rightarrow (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})_M, \end{aligned} \right\} \quad (9)$$

or, expressing the same atomic displacements as from integral initial positions relative to axes  $A$  to final positions relative to axes  $M$ ,

$$\left. \begin{aligned} (0, 0, 0)_A &\rightarrow (0, 0, 0)_M, \\ (\frac{1}{2}, \frac{1}{2}, 0)_A &\rightarrow (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})_M, \\ (\frac{1}{2}, 0, \frac{1}{2})_A &\rightarrow (1, 0, 0)_M, \\ (0, \frac{1}{2}, \frac{1}{2})_A &\rightarrow (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})_M. \end{aligned} \right\} \quad (10)$$

The correspondence in (10) between the initial positions referred to axes  $A$ , and the final positions referred to axes  $M$ , of the four atoms defining a primitive unit cell can be expressed alternatively by a linear relation of the type

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}_M = (\tau) \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix}_A \quad (11)$$

where  $\tau$  is the matrix of a relation which involves change of axis, change of lattice parameter, and transformation displacement. This relation given in (11) applies to the movement of every atom, since the deformation is homogeneous. The components of the matrix  $\tau$  can

be determined by solving (11) for the points whose transformation displacements have already been determined, and are listed in (10). We obtain

$$\tau = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}.$$

We can verify the generality of the matrix  $\tau$  by applying it to the general co-ordinate form of the face-centred cubic structure, i.e. to  $(\frac{1}{2}n_1, \frac{1}{2}n_2, \frac{1}{2}n_3)_A$ , where  $n_1 + n_2 + n_3$  is even. We have

$$\tau \times \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{2}n_2 \\ \frac{1}{2}n_3 \end{pmatrix}_A = \frac{1}{2} \begin{pmatrix} n_1 + n_3 \\ n_1 - n_3 \\ n_2 \end{pmatrix}_M.$$

Now  $n_1 + n_3$  and  $n_1 - n_3$  are like integers, and, since  $n_1 + n_2 + n_3$  is even,  $n_1 + n_3$  and  $n_2$  are like, i.e.

$$\frac{1}{2} \cdot \begin{pmatrix} n_1 + n_3 \\ n_1 - n_3 \\ n_2 \end{pmatrix}_M \equiv \begin{pmatrix} \frac{1}{2}\nu_1 \\ \frac{1}{2}\nu_2 \\ \frac{1}{2}\nu_3 \end{pmatrix}_M.$$

This verifies that the matrix  $\tau$  defines the relation between co-ordinate numbers in the two structures.

We may note that  $\tau$  could have been derived directly from (7) as the nearest integral matrix to the matrix  $\frac{a}{c}(M/A)$ , since it is obvious that as it has to connect integral co-ordinate numbers its components themselves must be integral.

### 5. The tetragonal axis in martensite

So far, the tetragonality of martensite has been neglected; however, this is very small ( $c/\alpha$  is never greater than 1.07) and so does not affect the components of  $\tau$  as previously derived. If, for example,  $M_z$  is assumed to be the unique axis, then (6) becomes modified to

$$\begin{pmatrix} x\alpha \\ y\alpha \\ zc \end{pmatrix}_M = (M/A)_{c/\alpha} \cdot \begin{pmatrix} xa \\ ya \\ za \end{pmatrix}_A, \quad (6a)$$

where the matrix  $(M/A)_{c/\alpha}$  depends on the axial ratio of the martensite and so on the carbon content of the steel under consideration.

On incorporating the lattice parameters into the matrix we obtain the analogue of (7),

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}_M = (M/A)'_{c/\alpha} \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix}_A. \quad (7a)$$

For all ranges of carbon content, the nearest integral matrix to  $(M/A)'_{c/\alpha}$  is still  $\tau$ ; similar results are obtained if  $M_x$  or  $M_y$  is assumed to be the unique axis.

The question as to which of the martensite axes becomes the unique axis is decided by the original assumption of a particular lattice relationship between the original and final phases, eight of the possible

relations giving rise to a structure with  $M_x$  as the tetragonal axis, eight giving  $M_y$ , and eight  $M_z$ . To identify the unique axis for the particular lattice relationship which we have assumed, we consider the movement of the carbon atoms. In austenite the carbon atom sites form a face-centred cubic lattice which interpenetrates that of the iron atoms (Petch, 1942), and in martensite they form a body-centred tetragonal lattice interpenetrating that of the iron atoms (Petch, 1943). This relation between the initial and final arrangements of the carbon atoms is most readily explained if we assume that they undergo the same homogeneous deformation as the iron atoms, i.e. that the final position referred to axes  $M$  of any carbon atom is derived from its initial position referred to axes  $A$  by the operation of the matrix  $\tau$ .

On the basis of this assumption, any carbon atom whose original co-ordinates are known can be assigned final co-ordinates relative to axes  $M$ , and the form of the co-ordinates in  $M$  identifies the tetragonal axis immediately because it is known from the work of Petch (1943) that the carbon atoms are situated at the midpoints of the long edges of the tetragonal unit cells.

The general co-ordinate form of a carbon atom site in austenite is  $(\frac{1}{2}n_1 + \frac{1}{2}, \frac{1}{2}n_2 + \frac{1}{2}, \frac{1}{2}n_3 + \frac{1}{2})_A$ . This is transferred by the operation of  $\tau$  to

$$\tau \cdot \begin{pmatrix} \frac{1}{2}n_1 + \frac{1}{2} \\ \frac{1}{2}n_2 + \frac{1}{2} \\ \frac{1}{2}n_3 + \frac{1}{2} \end{pmatrix}_A = \tau \cdot \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{2}n_2 \\ \frac{1}{2}n_3 \end{pmatrix}_A + \tau \cdot \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_A = \begin{pmatrix} \frac{1}{2}\nu_1 \\ \frac{1}{2}\nu_2 \\ \frac{1}{2}\nu_3 \end{pmatrix}_M + \begin{pmatrix} 1 \\ 0 \\ \frac{1}{2} \end{pmatrix}_M,$$

i.e. any carbon atom site in martensite is obtained by a

translation vector  $\begin{pmatrix} 1 \\ 0 \\ \frac{1}{2} \end{pmatrix}_M$  from any iron atom. If the

iron atom is at the corner of a cube, then the corresponding carbon site is half-way along a cell edge in the  $M_z$  direction; if the iron atom is in the body-centred position, then the carbon site is at the face centre of a face perpendicular to the  $M_z$  direction. In either case, the  $M_z$  axis is immediately distinguished as the unique tetrad axis for the particular case we are considering. We see, therefore, that the tetragonality of martensite arises as a necessary consequence of the assumption that the displacements of the iron and carbon atoms constitute a common homogeneous deformation.

It may be noted, by reference to the stereogram, that the unique axis coincides very closely with a co-ordinate axis of the face-centred cubic structure, and this provides a simple method for identifying it.

### 6. Calculation of the transformation strain

We have dealt so far with matrices which transform atomic co-ordinates or co-ordinate numbers from one axis-system to another. To derive an expression for the magnitude of the atomic displacements during the transformation we must consider the initial and final positions of the atoms relative to the same system of

co-ordinates. Thus if  $(xa, ya, za)_I$  and  $(x'a, y'a, z'a)_I$  are the original and final positions respectively of an atom referred to axes  $I$  (which are convenient for our present purpose), there is a relation between them of the form

$$\begin{pmatrix} x'a \\ y'a \\ z'a \end{pmatrix}_I = \begin{pmatrix} 1 + \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & 1 + \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & 1 + \sigma_{zz} \end{pmatrix} \cdot \begin{pmatrix} xa \\ ya \\ za \end{pmatrix}_I, \quad (12)$$

where the matrix  $\sigma$ , which refers only to atomic movements, is called the strain matrix.

In order to evaluate  $\sigma$  from (12) we proceed as follows.

The co-ordinates referred to axes  $A$  of the point  $(xa, ya, za)_I$  are given by

$$\begin{pmatrix} xa \\ ya \\ za \end{pmatrix}_A = (A/I) \cdot \begin{pmatrix} xa \\ ya \\ za \end{pmatrix}_I, \quad (13)$$

where  $(A/I)$ , the matrix of the axis transformation from axes  $I$  to axes  $A$ , is obtained from the reverse axis transformation  $(I/A)$  which has already been evaluated, by simple interchange of rows and columns.

The co-ordinate numbers of the atom referred to axes  $A$  are thus known; by operating with the matrix  $\tau$  we can obtain from these the co-ordinate numbers of the atom relative to axes  $M$  after the phase transformation has taken place, since

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_M = \tau \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix}_A. \quad (14)$$

The final co-ordinates of the atom referred to axes  $I$ ,  $(x'a, y'a, z'a)_I$ , are now obtained by the further axis transformation  $(I/M)$  given by

$$\begin{pmatrix} x'a \\ y'a \\ z'a \end{pmatrix}_I = (I/M)_{c/a} \cdot \begin{pmatrix} x'a \\ y'a \\ z'a \end{pmatrix}_M, \quad (15)$$

or, if we consider co-ordinate numbers only,

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_I = (I/M)'_{c/a} \cdot \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_M, \quad (16)$$

where  $(I/M)'_{c/a}$  incorporates the lattice parameters into  $(I/M)_{c/a}$ .

On combining (13), (14) and (16) we obtain

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_I = (I/M)'_{c/a} \cdot \tau \cdot (A/I) \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix}_I, \quad (17)$$

and, on comparing (12) and (17),

$$\sigma = (I/M)'_{c/a} \cdot \tau \cdot (A/I). \quad (18)$$

This equation enables us to evaluate  $\sigma$  for any particular carbon content, since each of the components

on the right-hand side is known, e.g. for the maximum possible carbon content of 1.7%,

$$a = 3.607 \text{ \AA}, \quad c = 3.039 \text{ \AA}, \quad \alpha = 2.839 \text{ \AA}, \quad c/\alpha = 1.070,$$

and the strain matrix is

$$\sigma_{1.7\%C} = \begin{pmatrix} 1.062 & 0 & 0.149 \\ 0.152 & 0.987 & 0.215 \\ 0 & 0 & 0.996 \end{pmatrix}.$$

For zero carbon content

$$\sigma_{0\%C} = \begin{pmatrix} 1.070 & 0 & 0.189 \\ 0.189 & 0.983 & 0.268 \\ 0 & 0 & 0.983 \end{pmatrix}.$$

For carbon contents between the above two limiting values, the components of the strain matrix all vary continuously with carbon content, and three of these components are zero for all compositions.

## 7. Properties of the strain tensor

The quantity

$$S = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix},$$

known as the strain tensor, represents the magnitude of the atomic movements referred to the co-ordinate system  $I$ . From the numerical values of  $\sigma$  it will be seen that the components of  $S$  are all finite, and hence that  $S$  has different properties from an infinitesimal strain tensor, where the squares and products of components can be neglected in comparison with the components themselves.

Thus it is an important feature of  $S$  that the various components or combinations of them have no independent physical significance, as is the case with infinitesimal strain. In particular,  $S$  cannot be decomposed into a symmetric tensor and a rigid-body rotation. Any decomposition of  $S$  is purely formal, and has no physical significance.

It is to be observed that, for all carbon contents,

$$\sigma_{zx} = \sigma_{zy} = 0, \quad (19a)$$

$$\sigma_{xy} = 0. \quad (19b)$$

Equation (19a) implies that there is no shear in the  $z$  direction, i.e. that the  $(111)_\gamma$  plane of atoms remains unchanged in direction during the atomic movements. The additional equation (19b) implies that the  $[1\bar{1}0]_\gamma$  direction of atoms also remains unchanged in direction.

It follows from the lattice relationships

$$(111)_\gamma \parallel (101)_\alpha, \quad [1\bar{1}0]_\gamma \parallel [1\bar{1}\bar{1}]_\alpha,$$

that the atoms which before transformation constitute the  $(111)_\gamma$  plane and  $[1\bar{1}0]_\gamma$  direction respectively, are the same atoms which after transformation constitute the  $(101)_\alpha$  plane and the  $[1\bar{1}\bar{1}]_\alpha$  direction respectively. Kurdjumow & Sachs (1930) implicitly assumed this



identity of the atoms which constitute the plane and direction which define the lattice relationship, and for this reason their picture of the atomic movements is consistent with the strain tensor developed above. It will be seen that in the present treatment, the assumption of Kurdjumow & Sachs regarding the identity of the atoms has been justified rigorously on the basis of the assumption of minimum distortion of a unit cell in the transformation process.

### 8. The habit plane

The habit plane of the martensite plate has been defined as the plane delineated by the observable midrib. However, as will be observed from Fig. 1, the great majority of the surface boundary of the plate is parallel to the habit plane, and it is therefore likely that surface-energy considerations are responsible for the selection of the particular habit plane which is adopted.

The suggestion is advanced that the selection of the plane  $\{225\}_\gamma$  as the habit plane for martensite having carbon contents less than 1.4% is due to the fact that, as will be shown, this plane undergoes no change in direction during the transformation. It is obvious that if the boundary plane itself underwent a large change of direction during the transformation, large-scale plastic distortion would be necessary for the surrounding austenite to accommodate the movement, and this arrangement of the plate is therefore energetically unfavourable.

The distortion represented by a finite non-symmetric strain tensor such as  $S$  is, in general, such that there are three planes which do not change in direction (proper planes). These three planes are not mutually orthogonal and so cannot conveniently be used to define a new system of reference axes, although they do define three oblique axes along which there are only extensions or contractions, these completely specifying the transformation.

Given a particular strain tensor,  $S$ , we can identify the proper planes as follows.

Any plane of the original structure is given by the equation

$$Ax + By + Cz + D = 0. \quad (20)$$

To find the equation satisfied by the points of this plane after the transformation has occurred, we substitute for  $x, y, z$  in terms of  $x', y', z'$ , where  $(x, y, z), (x', y', z')$  are related by the strain matrix  $\sigma$ , i.e.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \sigma \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \quad (21)$$

or rather by

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \sigma^{-1} \cdot \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}, \quad (22)$$

where  $\sigma^{-1}$  is the inverse matrix to  $\sigma$ .

On substituting from (22), and on collecting terms, (20) becomes

$$\begin{aligned} & \{(1 + \sigma_{yy})(1 + \sigma_{zz})A - \sigma_{yx}(1 + \sigma_{zz})B\}x' \\ & + (1 + \sigma_{xx})(1 + \sigma_{zz})By' + \{-\sigma_{xz}(1 + \sigma_{yy})A \\ & - [\sigma_{yz}(1 + \sigma_{xx}) + \sigma_{zx}\sigma_{yx}]B \\ & + (1 + \sigma_{xx})(1 + \sigma_{yy})C\}z' + D = 0. \end{aligned} \quad (23)$$

We now wish to introduce the condition that the plane is to remain unchanged in direction during the transformation, i.e. that (20) and (23) represent parallel planes. The appropriate condition is that the coefficients of  $x, y, z$  and  $x', y', z'$  in the two equations shall be related by the same constant of proportionality, i.e. that if

$$\left. \begin{aligned} & (1 + \sigma_{yy})(1 + \sigma_{zz})A - \sigma_{yx}(1 + \sigma_{zz})B = \lambda A, \\ & (1 + \sigma_{xx})(1 + \sigma_{zz})B = \lambda B, \\ & -\sigma_{xz}(1 + \sigma_{yy})A - [\sigma_{yz}(1 + \sigma_{xx}) + \sigma_{zx}\sigma_{yx}]B \\ & + (1 + \sigma_{xx})(1 + \sigma_{yy})C = \lambda C. \end{aligned} \right\} \quad (24)$$

For the three equations (24) to be mutually consistent, the constant of proportionality,  $\lambda$ , must satisfy the cubic equation

$$\begin{vmatrix} (1 + \sigma_{yy})(1 + \sigma_{zz}) - \lambda & & & \\ & -\sigma_{yx}(1 + \sigma_{zz}) & & \\ & & 0 & \\ 0 & & & (1 + \sigma_{xx})(1 + \sigma_{zz}) - \lambda \\ & & & & 0 \\ -\sigma_{xz}(1 + \sigma_{yy}) & & & & \\ & & & -[\sigma_{yz}(1 + \sigma_{xx}) + \sigma_{zx}\sigma_{yx}] & \\ & & & & (1 + \sigma_{xx})(1 + \sigma_{yy}) - \lambda \end{vmatrix} = 0. \quad (25)$$

Each of the roots of (25) will therefore determine one of the required proper planes on substitution into (24).

On inserting the numerical values of  $\lambda$  into these calculations it is found that, for all carbon contents, one of the planes which does not change in direction during the transformation is the plane  $(111)_\gamma$ . (This result can be seen directly from (19a).) A second solution gives, for all carbon contents, a plane lying within  $1^\circ$  of  $(111)_\gamma$  and becoming coincident with it for zero carbon content. The third root for  $\lambda$  defines a plane which lies within  $1\frac{1}{2}^\circ$  of  $(225)_\gamma$ .

The fact that the plane  $(111)_\gamma$  remains unchanged in direction during the transformation is consistent with the observation that in very low-carbon martensite, in which the habit plane is needle-like rather than plate-like, the needles group themselves into plates which delineate octahedral planes. The third solution provides that the habit plane for higher carbon contents up to 1.4% is a plane which undergoes no change in direction. Two questions remain outstanding, namely, the reason for the choice of the  $\{225\}_\gamma$  habit in preference to an octahedral habit, since both have been shown to satisfy

the condition of undergoing no directional change, and, secondly, the condition which determines the occurrence of the  $\{259\}_\gamma$  habit in martensite containing more than 1.4% carbon. Further work on the present lines may lead to the appreciation of a more general condition which determines the habit plane, but it is at least an interesting property of the habit plane over a very wide range of carbon concentrations which the present investigation has brought to light.

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## Short Communications

*Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Rapid publication will be easier if the contributions are without illustrations.*

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**The space group of phenanthrene.** By B. S. BASAK, *Indian Association for the Cultivation of Science, 210 Bowbazar Street, Calcutta, India*

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Phenanthrene is the parent body of a series of important organic compounds, namely, sterols and others, the structures and stereochemical pictures of which are still the subject of controversy in organic chemistry. It is also a member of a series of compounds of similar structural formulae, e.g. naphthalene, anthracene, chrysene, pyrene, etc., whose structures have already been determined. The main difficulty about this substance is to obtain single crystals of convenient dimensions. On the other hand, it possesses the advantage, in common with the above compounds, that all the atoms of the molecule are of the same scattering power (except, of course, hydrogen, the scattering power of which may fairly be neglected). The most difficult part of the structure determination by the Fourier synthesis method, namely, the determination of the signs of Fourier terms, can therefore be done by the algebraical method of Banerjee (1933). A few tolerably good crystals were obtained from a solution of a mixture of acetone and alcohol, and hence an attempt at a complete determination of the structure has been undertaken.

Phenanthrene has previously been studied by Mark & Hengstenberg (1929), who found the space group to be  $C_{2h}^2-P2_1/c$  with four molecules in the unit cell. We have taken rotation photographs about the three crystallographic axes and have found the following values for axial lengths and angles:

$$a = 8.57 \text{ \AA.}, \quad b = 6.11 \text{ \AA.}, \quad c = 9.47 \text{ \AA.}, \quad \beta = 97^\circ 30'.$$

There are two molecules per unit cell.

Overexposed photographs about the  $c$  axis from very clear crystals failed to reveal any faint layer line in between the main layer lines as noted by Mark &

Hengstenberg (1929). Oscillation and Weissenberg photographs about the three axes have shown that extinction occurs only for odd orders of  $(0k0)$  planes; hence the possible space groups are  $C_2^2-P2_1$  or  $C_{2h}^2-P2_1/m$ .

Now since there are two molecules per unit cell, there can be only two possible orientations for the phenanthrene molecule if the space group is  $C_{2h}^2-P2_1/m$ , the existence of a molecular centre of symmetry being impossible. One orientation is with the molecular plane coincident with the plane of symmetry, in which case the  $(020)$  reflexion will be very strong and subsequent orders will decrease uniformly but slowly. The experimental evidence is against this, the  $(020)$  being moderately strong,  $(040)$  very weak and  $(060)$  stronger than  $(040)$ . The only other possible orientation is with the plane of the molecule symmetrically at right angles to the plane of symmetry. But this arrangement also is not possible from steric considerations, assuming a planar configuration for the molecule and taking 1.41 Å. as the C-C distance; the length of the molecule becomes too long to be accommodated in the unit cell. From these considerations the space group  $C_{2h}^2-P2_1/m$  is discarded and the crystal is assigned the space group  $C_2^2-P2_1$ . The structure factors of a large number of different planes have been determined experimentally, and a complete determination of the structure is being attempted by the help of Fourier analysis.

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