

NYO-756

I

ATOMIC DISPLACEMENTS AND CRYSTALLOGRAPHIC  
MECHANISM IN DIFFUSIONLESS TRANSFORMATION OF GOLD-CADMIUM  
CRYSTALS CONTAINING 47.5 ATOMIC PERCENT CADMIUM

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ABSTRACT

The atomic displacements and crystallographic mechanism in diffusionless transformation of Au-Cd single crystals containing 47.5 atomic percent Cd were investigated. The alloy transforms from an ordered body-centered cubic structure ( $\beta_1$ ) on cooling to about 60°C to an orthorhombic structure ( $\beta'$ ). The reverse transformation from  $\beta'$  to  $\beta_1$  takes place when the alloy is heated to about 80°C. The lattice parameters of both phases were determined by X-ray measurements to be:  $\beta_1$ ,  $a = 3.3165 \pm 0.0005$  kX units (corrected to room temperature);  $\beta'$ ,  $a = 3.1476 \pm 0.0005$ ,  $b = 4.7549 \pm 0.0005$ ,  $c = 4.8546 \pm 0.0005$  kX units.

Atomic displacements involved in the transformation were discussed and transformation matrices were derived. The crystallographic mechanism of the transformation was experimentally evaluated as a  $(\bar{3}31)_{\beta_1} [323]_{\beta_1}$  simple homogeneous shear of about 3 degrees ( $\tan \gamma = 0.05$ ), plus a possible contraction of the b edge of the orthorhombic cell by about 0.015 kX units. The lattice parameters of the orthorhombic phase calculated according to this crystallographic mechanism are in almost exact agreement with those directly obtained by X-ray measurements.

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## I. INTRODUCTION

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Diffusionless transformation in metals and alloys has been a widely studied subject of both theoretical and practical interest since a decade ago. Experimental investigations of the problem have been reported in literature on Fe-C<sup>(1,2,3,4)\*</sup>, Fe-Ni<sup>(4,5,6,7)</sup>, Fe-Mn<sup>(8)</sup>, Cu-Al<sup>(9,10)</sup>, Cu-Zn<sup>(11)</sup>, Cu-Sn<sup>(11)</sup>, Li<sup>(12)</sup>, Li-Mg<sup>(12)</sup>, Co<sup>(13)</sup>, Zr<sup>(14)</sup>, and In-Tl<sup>(19)</sup>.

The diffusionless transformation in single crystals of Au-Cd alloys containing 47.5 atomic percent Cd has been studied by Chang and Read<sup>(15)</sup>. The purpose of this paper is to determine the crystallographic mechanism and atomic displacements involved in diffusionless transformation of this alloy.

## II. CRYSTAL STRUCTURE

The Au-Cd alloy containing 47.5 atomic percent Cd undergoes a diffusionless transformation from an ordered body-centered cubic structure ( $\beta_1$ ) to an orthorhombic structure ( $\beta'$ ) when it is cooled to about 60°C, and the reverse transformation from  $\beta'$  to  $\beta_1$  takes place when the alloy is heated to about 80°C. The crystal structures of these phases have been studied by Ölander<sup>(16)</sup> and by Bystrom and Almin<sup>(17)</sup>, both using powdered samples. Single crystals of both phases were prepared by the author and their crystal structures were verified by means of back reflection Laue methods to be, respectively, of the CsCl type and of orthorhombic symmetry. The lattice parameters of both phases were determined by the author using single crystal oscillation method with CuK radiation reflecting from, respectively, the (411) plane of the ordered body-centered cubic phase and (400), (060), (006) planes of the orthorhombic phase. The results are compared with those of Bystrom and Almin<sup>(17)</sup> in Table I.

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\* References are at the end of the paper.

TABLE I. LATTICE PARAMETERS OF  
 $\beta_1$  AND  $\beta'$

$\beta_1$  . body-centered cubic, ordered, two atoms per unit cell  
 $\beta'$  . orthorhombic, four atoms per unit cell

Cell Edge	Author's, kX units		Bystrom & Almin, kX units
$\beta_1$ . $\alpha$ (cube edge)	$3.3165 \pm 0.0005$	$(25^\circ\text{C})^*$	$3.305 \pm 0.002$
$\beta'$ . a	$3.1476 \pm 0.0005$	$(25^\circ\text{C})$	$3.144 \pm 0.003^{**}$
b	$4.7549 \pm 0.0005$	$(25^\circ\text{C})$	$4.755 \pm 0.004$
c	$4.8546 \pm 0.0005$	$(25^\circ\text{C})$	$4.851 \pm 0.004$

\*Extrapolated to room temperature from two determinations,  $3.3259 \pm 0.0005$  kX units at  $149^\circ\text{C}$  and  $3.3203 \pm 0.0005$  kX units at  $78^\circ\text{C}$ .

\*\* The b and c cell edges given by Bystrom and Almin are interchanged in this paper so that the cell edge increases from a to b and to c.

### III. ATOMIC DISPLACEMENTS AND TRANSFORMATION MATRICES

The orientation relationships between  $\beta_1$  and  $\beta'$  as determined by Chang and Read<sup>(15)</sup> are:

$$\begin{aligned} (100)_{\beta_1} & \text{ parallel to } (100)_{\beta'} \quad . \text{ planes} \\ [\bar{1}\bar{1}\bar{1}]_{\beta_1} & \text{ parallel to } [\bar{1}\bar{1}0]_{\beta'} \quad . \text{ directions} \end{aligned} \quad (1).$$

The orientation relationships shown above indicate that one of the cube edges of  $\beta_1$  is approximately parallel to the a-edge of  $\beta'$ , and two face diagonals of  $\beta_1$  are approximately parallel, respectively, to the b- and c- edges of  $\beta'$ , with a deviation of 1 to 1-1/2 degrees, which is about the limit of experimental error in orientation relationship determinations. These relationships can therefore, within the limits of experimental error, be expressed by the parallelism of three pairs of directions:

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$$\begin{aligned}
 [100]_{\beta_1} & \text{ parallel to } [100]_{\beta'} & I_x \\
 [01\bar{1}]_{\beta_1} & \text{ parallel to } [010]_{\beta'} & I_y \\
 [011]_{\beta_1} & \text{ parallel to } [001]_{\beta'} & I_z
 \end{aligned} \quad (2)$$

The three directions  $I_x$ ,  $I_y$  and  $I_z$  form a convenient set of intermediate rectangular axes of reference I, the relations of which to the  $\beta_1$  and  $\beta'$  phases are determined by the direction cosines between the corresponding axes. The direction cosines between the reference axes  $I_x$ ,  $I_y$  and  $I_z$  and the axes of  $\beta_1$  and  $\beta'$  phases are, according to equation (2), as follows:

$$\begin{array}{l}
 I - \beta_1 : \\
 \begin{array}{lll}
 l_1 = 1 & m_1 = 0 & n_1 = 0 \\
 l_2 = 0 & m_2 = \frac{1}{\sqrt{2}} & n_2 = -\frac{1}{\sqrt{2}} \\
 l_3 = 0 & m_3 = \frac{1}{\sqrt{2}} & n_3 = \frac{1}{\sqrt{2}}
 \end{array}
 \end{array} \quad (3)$$

$$\begin{array}{l}
 I - \beta' : \\
 \begin{array}{lll}
 l_1' = 1 & m_1' = 0 & n_1' = 0 \\
 l_2' = 0 & m_2' = 1 & n_2' = 0 \\
 l_3' = 0 & m_3' = 0 & n_3' = 1
 \end{array}
 \end{array} \quad (4)$$

We shall now use the above relations to refer to axes  $\beta'$  the coordinates of an atomic site known relative to axes  $\beta_1$ , following the method of Jaswon and Wheeler<sup>(18)</sup>.

Consider the atomic site

$$(h\alpha, k\alpha, l\alpha)_{\beta_1}$$

where  $h, k, l$  are coordinate numbers,  $\alpha$  the lattice parameter of  $\beta_1$  (see Table I), and the subscript  $\beta_1$  indicate the axes of reference. If the coordinates of this same atomic site relative to axes  $\beta'$  are  $(h'a, k'b, l'c)_{\beta'}$ , where  $h', k', l'$  are coordinate numbers,  $a, b$  and  $c$  are the lattice parameters of  $\beta'$  (see Table I), and the subscript  $\beta'$  refers to the axes of reference, then the following relation holds:

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$$\begin{pmatrix} h' \\ k' \\ l' \end{pmatrix}_{\beta'} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \cdot \begin{pmatrix} h \\ k \\ l \end{pmatrix}_{\beta_1} \quad (5)$$

or, expressing the relation between coordinate numbers instead of coordinates, it follows:

$$\begin{pmatrix} h' \\ k' \\ l' \end{pmatrix}_{\beta'} = \begin{pmatrix} \frac{\alpha}{a} & 0 & 0 \\ 0 & \frac{\alpha}{b\sqrt{2}} & -\frac{\alpha}{b\sqrt{2}} \\ 0 & \frac{\alpha}{c\sqrt{2}} & \frac{\alpha}{c\sqrt{2}} \end{pmatrix} \cdot \begin{pmatrix} h \\ k \\ l \end{pmatrix}_{\beta_1} \quad (6)$$

Substituting the numerical values of  $\alpha$ ,  $a$ ,  $b$ , and  $c$  (see Table I) into equation (6), it follows:

$$\begin{pmatrix} h' \\ k' \\ l' \end{pmatrix}_{\beta'} = M \begin{pmatrix} h \\ k \\ l \end{pmatrix}_{\beta_1}, \quad M = \begin{pmatrix} 1.049 & 0 & 0 \\ 0 & 0.492 & -0.492 \\ 0 & 0.482 & 0.482 \end{pmatrix} \quad (7)$$

where  $M$  is the matrix of transformation.

The coordinates of an atom in  $\beta_1$ , relative to axes  $\beta_1$ , are of the form  $(\frac{1}{2}n_1\alpha, \frac{1}{2}n_2\alpha, \frac{1}{2}n_3\alpha)$ , where  $n_1$ ,  $n_2$  and  $n_3$  are integers. Because the structure of  $\beta_1$  is CsCl type, the three integers must be either all odd or all even. If the sites with  $n_1$ ,  $n_2$ ,  $n_3$  all even belong to Au atoms, those with  $n_1$ ,  $n_2$ ,  $n_3$  all odd must belong to Cd atoms.

The exact locations of the atoms in the orthorhombic  $\beta'$  unit cell have not been established. Bystrom and Almin<sup>(17)</sup> reported that the unit cell contains four atoms with two Au atoms located approximately at  $0, 0, 0$  and  $0, 1/2, 5/8$  and two Cd atoms located approximately at  $1/2, 0, 1/2$  and  $1/2, 1/2, 1/8$ . Since the exact positions of these atoms in the unit cell are now known, it is reasonable, for purposes of simplification, to describe the orthorhombic cell as face-centered with two Au atoms located approximately at  $0, 0, 0$  and  $0, 1/2, 1/2$  and two Cd atoms located approximately at  $1/2, 0, 1/2$  and  $1/2, 1/2, 0$ . The coordinates of an atom in  $\beta'$  referred to

axes  $\beta'$  are then of the form  $(\frac{1}{2}m_1a, \frac{1}{2}m_2b, \frac{1}{2}m_3c)$  where  $m_1, m_2, m_3$  are integers and  $(m_1 + m_2 + m_3)$  is even. The sites with  $m_1 = \text{even}$  belong to Au atoms, and those with  $m_1 = \text{odd}$  belong to Cd atoms.

We shall now consider the atomic displacements involved in generating the  $\beta'$  structure from the  $\beta_1$  structure, assuming 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  $\beta_1$ . Let the coordinate numbers of the four atoms defining a primitive unit cell of  $\beta_1$  be:

$$(0, 0, 0)_{\beta_1}, \quad (0, 1, 0)_{\beta_1}, \quad (1/2, 1/2, 1/2)_{\beta_1}, \quad (1/2, 1/2, -1/2)_{\beta_1}$$

where  $(0, 0, 0)_{\beta_1}$  and  $(0, 1, 0)_{\beta_1}$  are Au atoms and  $(1/2, 1/2, 1/2)_{\beta_1}$ ,  $(1/2, 1/2, -1/2)_{\beta_1}$  are Cd atoms. Following the method adopted by Jaswon and Wheeler (18) and

assuming that, of the many possible distortions of a primitive unit cell of  $\beta_1$  by which the  $\beta'$  structure could be generated, the one which actually occurs is the smallest, we immediately identify the displacements of the four atoms in question during the

$\beta_1 \rightarrow \beta'$  transformation as being:

$$\begin{array}{llll} (0, 0, 0)_{\beta_1} & \longrightarrow & (0, 0, 0)_{\beta'} & \text{Au-atom} \\ (0, 1, 0)_{\beta_1} & \longrightarrow & (0, 1/2, 1/2)_{\beta'} & \text{Au-atom} \\ (1/2, 1/2, 1/2)_{\beta_1} & \longrightarrow & (1/2, 0, 1/2)_{\beta'} & \text{Cd-atom} \\ (1/2, 1/2, -1/2)_{\beta_1} & \longrightarrow & (1/2, 1/2, 0)_{\beta'} & \text{Cd-atom} \end{array} \quad (8)$$

The correspondence in equation (8) between the initial positions referred to axes  $\beta_1$  and the final positions referred to axes  $\beta'$ , of the four atoms defining a primitive unit cell can be expressed alternatively by a linear relation of the type:

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$$\begin{pmatrix} h' \\ k' \\ l' \end{pmatrix}_{\beta'} = (\mathcal{T}) \cdot \begin{pmatrix} h \\ k \\ l \end{pmatrix}_{\beta_1}, \quad \mathcal{T} = \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & 1 & 1 \end{pmatrix} \quad (9)$$

where  $(\mathcal{T})$  is the matrix of a relation which involves change of axis, change of lattice parameter, and transformation displacement. The relation given in equation (9) applies to the movement of every atom, since the deformation is homogeneous. This relation can be easily converted to transformation matrices for both direction transformations and plane transformations. The matrix  $(\mathcal{T})$  is in fact the direction transformation matrix from  $\beta_1$  to  $\beta'$ . Thus we have:

$$\begin{pmatrix} h' \\ k' \\ l' \end{pmatrix}_{\beta'} \longleftrightarrow \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} h \\ k \\ l \end{pmatrix}_{\beta_1} \quad (10)$$

and, using the inverse matrix, we have:

$$\begin{pmatrix} h \\ k \\ l \end{pmatrix}_{\beta_1} \longleftrightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & -1 & 1 \end{pmatrix} \cdot \begin{pmatrix} h' \\ k' \\ l' \end{pmatrix}_{\beta'} \quad (11)$$

where  $[h', k', l']_{\beta'}$  are the indices of a given direction of  $\beta'$  transformed from the direction  $[h, k, l]_{\beta_1}$  of  $\beta_1$ , and vice versa.

A similar operation yields the following plane transformation matrices:

$$\begin{pmatrix} h' \\ k' \\ l' \end{pmatrix}_{\beta'} \longleftrightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} h \\ k \\ l \end{pmatrix}_{\beta_1} \quad (12)$$

and

$$\begin{pmatrix} h \\ k \\ l \end{pmatrix}_{\beta_1} \longleftrightarrow \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & -1 & 1 \end{pmatrix} \cdot \begin{pmatrix} h' \\ k' \\ l' \end{pmatrix}_{\beta'} \quad (13)$$

where  $(h', k', l')_{\beta'}$  are the indices of a given plane of  $\beta'$  transformed from the  $(h, k, l)_{\beta_1}$  plane of  $\beta_1$ , and vice versa.

#### IV. Crystallographic Mechanism of the $\beta_1 \rightarrow \beta'$ Transformation

The atomic displacements and transformation matrices discussed in the previous section describe only the initial and final stages of transformation but not the actual path taken by the crystal in its transformation from  $\beta_1$  to  $\beta'$ , or vice versa. The actual crystallographic mechanism of the  $\beta_1 \rightarrow \beta'$  transformation will be derived in this section directly from experimental data. It will be desirable, however, to describe some of the physical characteristics of the transformation<sup>(15)</sup> which lead to the determination of the crystallographic mechanism:

(a) The transformation takes place typically by the slow movement of an interface between the two phases,  $\beta_1$  and  $\beta'$ .

(b) The transformation takes place in a well-grown and annealed  $\beta_1$  single crystal by the formation of a  $\beta'$  plate at one end of the specimen, thereby forming an interface, and by slow movement of this interface to the other end of the specimen. On reverse transformation from  $\beta'$  to  $\beta_1$ , the opposite happens.

(c) An optically flat surface of the  $\beta_1$  crystal transforms into an optically flat surface of the  $\beta'$  crystal by a mechanism very similar to simple homogeneous shear.

(d) It is possible to maintain the interface near the middle of the specimen by temperature control. On one side of the interface there is a single crystal of  $\beta_1$  and on the other side of the interface there is a single crystal of  $\beta'$  transformed from  $\beta_1$ .

(e) The slow moving interface has been previously identified<sup>(15)</sup> to be a (331) type plane of the  $\beta_1$  phase. The interface moves on transformation at a velocity (about 0.01 to 0.1 mm/sec.) almost directly proportional to the rate of cooling (or heating) of the specimen.

Single crystals of  $\beta_1$  with two flat surfaces across the length of the specimen were therefore prepared. The interface between  $\beta_1$  and  $\beta'$  was maintained near the middle of the specimen. The two flat surfaces of  $\beta_1$ , A and B, transform, respectively, to two flat surfaces, A' and B', of  $\beta'$ . If the mechanism of

transformation is a simple homogeneous shear, it should be possible to determine the plane of shear, direction of shear, and degree of shear by measuring the angular distortions involved in going from A to A' and from B to B'. The angular differences between A and A' and between B and B' were therefore measured by means of a two circle optical goniometer accurate to within 2 to 3 minutes of arc. The shear plane, shear direction, and degree of shear were found with the aid of stereographic projection by a method similar to that used by Greninger and Troiano (7). The results of two separate determinations are shown in Table II.

Table II. Determination of Crystallographic Mechanism of  $\beta_1$  ---  $\beta'$  Transformation

<u>Crystal No. 2</u>	( A' - A )	( B' - B )
Horizontal Circle	-67 $\pm$ 2 Minutes	-18 $\pm$ 2 Minutes
Vertical Circle	-20 $\pm$ 1 Minutes	-15 $\pm$ 1 Minutes
Shear plane $(\bar{3}31)_{\beta_1}$ .	Shear direction $[323]_{\beta_1}$ .	Degree of shear $\gamma_0 = 3^\circ 2'$ ( $\tan \gamma_0 = .053$ )

Crystal No. 7

Horizontal Circle	+ 33 $\pm$ 1 Minutes	+55 $\pm$ 1 Minutes
Vertical Circle	- 40 $\pm$ 1 Minutes	-89 $\pm$ 2 Minutes
Shear plane $(\bar{3}31)_{\beta_1}$ .	Shear direction $[323]_{\beta_1}$ .	Degree of shear $\gamma_0 = 2^\circ 45'$ ( $\tan \gamma_0 = .047$ )

The experimentally measured crystallographic mechanism of  $\beta_1$  ---  $\beta'$  transformation is therefore a simple homogeneous shear of the type  $(\bar{3}31)_{\beta_1} [323]_{\beta_1}$  by about 3 degrees.

V. Correlation of Experimentally Determined Shear Mechanism with Theoretical Calculations

According to the orientation relationships given by equation (2), the lattice point at  $(\alpha, \sqrt{2}\alpha, \sqrt{2}\alpha)$  referred to axes I before transformation becomes the lattice point ( a, b, c ) after transformation referred to the same axes I. The displacement of this lattice point due to transformation can therefore be calculated directly from

the orientation relationships and the lattice parameters of these two phases as follows: ( $\alpha$ , a, b, c see Table I)

$$\begin{aligned} U' &= a - \alpha = (a/\alpha - 1)\alpha \\ V' &= b - \sqrt{2}\alpha = (b/\alpha - \sqrt{2})\alpha \\ W' &= c - \sqrt{2}\alpha = (c/\alpha - \sqrt{2})\alpha \end{aligned} \quad (14)$$

On the other hand, knowing the shear mechanism we can calculate the displacements of the lattice point ( $\alpha$ ,  $\sqrt{2}\alpha$ ,  $\sqrt{2}\alpha$ ), that is,  $U'$ ,  $V'$  and  $W'$  independently without the knowledge of the lattice parameters of the  $\beta'$  phase. In other words, if  $U'$ ,  $V'$  and  $W'$  are known, we can calculate a, b and c according to equation (14). Thus it becomes possible to calculate the lattice parameters of the orthorhombic phase from the shear mechanism. Comparison of the calculated lattice parameters and experimental lattice parameters of the orthorhombic phase then provides a good check on the experimentally determined shear mechanism.

A set of reference axes is chosen such that the Y-axis is the shear direction, the Z-axis is the direction perpendicular to the shear plane, and the X-axis is the direction perpendicular to both Y and Z, that is,

$$\begin{aligned} X \text{ axis} & \quad [7 \quad 12 \quad \overline{15}] \beta_1 \\ Y \text{ axis} & \quad [3 \quad 2 \quad 3] \beta_1 \\ Z \text{ axis} & \quad [\overline{3} \quad 3 \quad 1] \beta_1 \end{aligned}$$

The experimental shear therefore corresponds to the following set of lattice displacements:

$$\begin{aligned} \frac{\partial u}{\partial x} &= 0, & \frac{\partial u}{\partial y} &= 0, & \frac{\partial u}{\partial z} &= 0, \\ \frac{\partial v}{\partial x} &= 0, & \frac{\partial v}{\partial y} &= 0, & \frac{\partial v}{\partial z} &= \tan \lambda_0 = 0.050 \\ \frac{\partial w}{\partial x} &= 0, & \frac{\partial w}{\partial y} &= 0, & \frac{\partial w}{\partial z} &= 0. \end{aligned} \quad (15)$$

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or

$$e_{xx} = \frac{\partial u}{\partial x} = 0, \quad e_{yz} = \frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} = 0.050, \quad \omega_x = \frac{1}{2} \left( \frac{\partial w}{\partial y} - \frac{\partial v}{\partial z} \right) = -0.025$$

$$e_{yy} = \frac{\partial v}{\partial y} = 0, \quad e_{zx} = \frac{\partial w}{\partial z} + \frac{\partial u}{\partial x} = 0, \quad \omega_y = \frac{1}{2} \left( \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x} \right) = 0, \quad (16)$$

$$e_{zz} = \frac{\partial w}{\partial z} = 0, \quad e_{xy} = \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} = 0, \quad \omega_z = \frac{1}{2} \left( \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) = 0.$$

Now we shall transform the strain components from reference axes X, Y, Z to other reference axes X', Y', Z' where X' = [100]<sub>β</sub>, Y' = [011]<sub>β</sub>, Z' = [011]<sub>β</sub> are the three directions parallel to, respectively, the a, b, c axes of the orthorhombic cell after transformation. The direction cosines between these axes are:

	X	Y	Z
	[ 7 12 15 ]	[ 3 2 3 ]	[ 3 3 1 ]
X' [100]	$l_1 = \frac{7}{\sqrt{418}}$	$m_1 = \frac{3}{\sqrt{22}}$	$n_1 = \frac{3}{\sqrt{19}}$
Y' [011]	$l_2 = \frac{27}{\sqrt{836}}$	$m_2 = -\frac{1}{\sqrt{44}}$	$n_2 = \frac{2}{\sqrt{38}}$
Z' [011]	$l_3 = -\frac{3}{\sqrt{836}}$	$m_3 = \frac{5}{\sqrt{44}}$	$n_3 = \frac{4}{\sqrt{38}}$

(17)

The components of strain referred to the new reference axes X', Y', Z' are then:

$$e_{x'x'} = l_1^2 e_{xx} + m_1^2 e_{yy} + n_1^2 e_{zz} + m_1 n_1 e_{yz} + n_1 l_1 e_{zx} + l_1 m_1 e_{xy}$$

$$e_{y'z'} = 2l_2 l_3 e_{xx} + 2m_2 m_3 e_{yy} + 2n_2 n_3 e_{zz} + (m_2 n_3 + m_3 n_2) e_{yz} + (n_2 l_3 + n_3 l_2) e_{zx} + (l_2 m_3 + l_3 m_2) e_{xy} \quad (18)$$

$$v_{z'} = l_1 v_x + m_1 v_y + n_1 v_z$$

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The displacements  $U'$ ,  $V'$ ,  $W'$  of a given lattice point  $(X', Y', Z')$  referred to the axes  $X'$ ,  $Y'$ ,  $Z'$  are, neglecting terms containing powers of  $X'$ ,  $Y'$ ,  $Z'$  above the first:

$$\begin{aligned} U' &= e_{x'x'} X' + 1/2 e_{x'y'} Y' + 1/2 e_{z'x'} Z' - v_z Y' + v_y Z' \\ V' &= 1/2 e_{x'y'} X' + e_{y'y'} Y' + 1/2 e_{y'z'} Z' - w_x Z' + w_z X' \\ W' &= 1/2 e_{z'x'} X' + 1/2 e_{y'z'} Y' + e_{z'z'} Z' - w_y X' + w_x Y' \end{aligned} \quad (19)$$

Combining equations (16), (17), (18) and (19), we get the following displacements of the lattice point  $(X' = \alpha, Y' = \sqrt{2}\alpha, Z' = \sqrt{2}\alpha)$ :

$$\begin{aligned} U' &= -0.0514\alpha \\ V' &= +0.0242\alpha \\ W' &= +0.0485\alpha \end{aligned} \quad (20)$$

Solving  $a$ ,  $b$ ,  $c$  from equations (14) and (20), we obtain the following calculated lattice parameters of the orthorhombic cell:

$$\begin{aligned} a &= 3.1460 \text{ kX units} \\ b &= 4.7704 \text{ kX units} \\ c &= 4.8510 \text{ kX units} \end{aligned}$$

The correspondence between the calculated and measured (by X-ray methods) lattice parameters of the orthorhombic cell is very good for the  $a$  and  $c$  axes and fair for the  $b$  axis. The comparison does not take into consideration any lattice readjustment, such as homogeneous contraction (or expansion) parallel to certain crystallographic directions, which might take place during transformation. Thus, a homogeneous contraction by 0.015 kX units along the  $b$ -axis of the orthorhombic cell will bring almost exact agreement between the calculated and measured lattice parameters of the orthorhombic phase.

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