Acta Cryst. (1951). **4**, 320

Atomic Displacements and Crystallographic Mechanism in Diffusionless Transformation of Gold–Cadmium Single Crystals containing 47·5 atomic percent Cadmium

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(*Received* 13 *November* 1950)

The atomic displacements and crystallographic mechanism in diffusionless transformation of Au–Cd single crystals containing 47·5 atomic percent Cd have been investigated. The alloy transforms from an ordered body-centered cubic structure (β_1) on cooling to about 60° C. to an orthorhombic structure (β'). The reverse transformation from β' to β_1 takes place when the alloy is heated to about 80° C. The lattice parameters of both phases, determined by X-ray measurements, are

$$\beta_1: \quad a = 3{\cdot}3165 \pm 0{\cdot}0005\ \text{kX.}$$

(corrected to room temperature);

$$\beta': \quad a = 3{\cdot}1476 \pm 0{\cdot}0005, \quad b = 4{\cdot}7549 \pm 0{\cdot}0005, \quad c = 4{\cdot}8546 \pm 0{\cdot}0005\ \text{kX.}$$

Atomic displacements involved in the transformation are discussed and transformation matrices are derived. The crystallographic mechanism of the transformation was experimentally evaluated as a $(\bar{3}31)_{\beta_1}$ $[323]_{\beta}$ simple homogeneous shear of about 3° ($\tan \gamma_0 = 0{\cdot}05$), 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.

1. Introduction

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 as follows:

Fe–C	Kurdjumow & Sachs, 1930; Smith & Mehl, 1942; Cohen, 1949; Wassermann, 1935.
Fe–Ni	Wassermann, 1935; Nishiyama, 1934; Mehl & Derge, 1937; Greninger & Troiano, 1949.
Fe–Mn	Troiano & McGuire, 1943.
Cu–Al	Greninger, 1939; Gridnev, 1938.
Cu–Zn	Greninger & Mooradian, 1938.
Cu–Sn	Greninger & Mooradian, 1938.
Li	Barrett & Trautz, 1948.
Li–Mg	Barrett & Trautz, 1948.
Co	Troiano & Tokich, 1948.
Zr	Burgers, 1934.
In–Tl	Smith, 1950.

The diffusionless transformation in single crystals of Au–Cd alloys containing 47·5 atomic percent Cd has been studied by Chang & Read (1950). The purpose of this paper is to determine the crystallographic mechanism and atomic displacements involved in diffusionless transformation of the alloy.

2. Crystal structure

The Au–Cd alloy containing 47·5 atomic percent Cd undergoes a diffusionless transformation from an ordered body-centred cubic structure (β_1) to an orthorhombic structure (β') when cooled to about 60° C., and the reverse transformation from β' to β_1 takes place when the alloy is heated to about 80° C. The crystal structures of these phases have been studied by Ölander (1932) and by Bystrom & Almin (1947), 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 of the CsCl type and of orthorhombic symmetry respectively. The lattice parameters of both phases were determined by the author using the single-crystal oscillation method with Cu K radiation reflected from the (411) plane of the ordered body-centered cubic phase and the (400), (060) and (006) planes of the orthorhombic phase. The results are compared with those of Bystrom & Almin (1947) in Table 1.

Table 1. *Lattice parameters of* β_1 *and* β'

β_1, body-centered cubic, ordered, two atoms per unit cell.
β', orthorhombic, four atoms per unit cell.

Cell edge	Chang (kX.)	Bystrom & Almin (kX.)
β_1, a (cube edge)	3·3165 ± 0·0005 (25° C.)*	3·305 ± 0·002
β', a	3·1476 ± 0·0005 (25° C.)	3·144 ± 0·003†
b	4·7549 ± 0·0005 (25° C.)	4·755 ± 0·004
c	4·8546 ± 0·0005 (25° C.)	4·851 ± 0·004

* Extrapolated to room temperature from two determinations, 3·3259 ± 0·0005 kX. at 149° C. and 3·3203 ± 0·0005 kX. at 78° C.

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

3. Atomic displacements and transformation matrices

The orientation relationships between β_1 and β', as determined by Chang & Read (1950), are:

$$\left.\begin{array}{l}(100)_{\beta_1} \text{ parallel to } (100)_{\beta'},\\ [\bar{1}\bar{1}1]_{\beta_1} \text{ parallel to } [\bar{1}\bar{1}0]_{\beta'}.\end{array}\right\} \tag{1}$$

These relationships indicate that one of the cube edges of β_1 is approximately parallel to the a edge of β', and two face diagonals of β_1 are approximately parallel, respectively, to the b and c edges of β', with a deviation of 1–1½°, 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:

$$\left.\begin{array}{lll}[100]_{\beta_1} \text{ parallel to } [100]_{\beta'} & I_x, \\ [01\bar{1}]_{\beta_1} \text{ parallel to } [010]_{\beta'} & I_y, \\ [011]_{\beta_1} \text{ parallel to } [001]_{\beta'} & I_z.\end{array}\right\} \tag{2}$$

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 β_1 and β' phases are determined by the direction cosines between the corresponding axes. The direction cosines between the references axes I_x, I_y and I_z and the axes of β_1 and β' phases are, according to equation (2), as follows:

$$\left.\begin{array}{llll}I(\beta_1): & l_1=1 & m_1=0 & n_1=0, \\ & l_2=0 & m_2=1/\sqrt{2} & n_2=-1/\sqrt{2}, \\ & l_3=0 & m_3=1/\sqrt{2} & n_3=1/\sqrt{2};\end{array}\right\} \tag{3}$$

$$\left.\begin{array}{llll}I(\beta'): & l'_1=1 & m'_1=0 & n'_1=0, \\ & l'_2=0 & m'_2=1 & n'_2=0, \\ & l'_3=0 & m'_3=0 & n'_3=1.\end{array}\right\} \tag{4}$$

We shall now use the above relations to refer to axes β' the co-ordinates of an atomic site known relative to axes β_1, following the method of Jaswon & Wheeler (1948). Consider the atomic site

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

where h, k, l are co-ordinate numbers, α the lattice parameter of β_1 (see Table 1), and the subscript β_1 indicates the axes of reference. If the co-ordinates of this same atomic site relative to axes β' are $(h'a, k'b, l'c)_{\beta'}$, where h', k', l' are co-ordinate numbers, a, b and c are the lattice parameters of β' (see Table 1), and the subscript β' refers to the axes of reference, then the following relation holds:

$$\begin{pmatrix} h'a \\ k'b \\ l'c \end{pmatrix}_{\beta'} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} h\alpha \\ k\alpha \\ l\alpha \end{pmatrix}_{\beta_1}, \tag{5}$$

or, expressing the relation between co-ordinate numbers instead of co-ordinates, it follows:

$$\begin{pmatrix} h' \\ k' \\ l' \end{pmatrix}_{\beta'} = \begin{pmatrix} \frac{\alpha}{a} & 0 & 0 \\ 0 & \frac{\alpha}{b}\frac{1}{\sqrt{2}} & -\frac{\alpha}{b}\frac{1}{\sqrt{2}} \\ 0 & \frac{\alpha}{c}\frac{1}{\sqrt{2}} & \frac{\alpha}{c}\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} h \\ k \\ l \end{pmatrix}_{\beta_1}. \tag{6}$$

Substituting the numerical values of α, a, b and c (see Table 1) in equation (6), it follows:

$$\begin{pmatrix} h' \\ k' \\ l' \end{pmatrix}_{\beta'} = M \begin{pmatrix} h \\ k \\ l \end{pmatrix}_{\beta_1}, \quad M = \begin{pmatrix} 1{\cdot}049 & 0 & 0 \\ 0 & 0{\cdot}492 & -0{\cdot}492 \\ 0 & 0{\cdot}482 & 0{\cdot}482 \end{pmatrix}, \tag{7}$$

where M is the matrix of transformation.

The co-ordinates of an atom in β_1 relative to axes β_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 β_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 gold atoms, those with n_1, n_2, n_3 all odd must belong to cadmium atoms.

The exact locations of the atoms in the orthorhombic β' unit cell have not been established. Bystrom & Almin (1947) reported that the unit cell contains four atoms with two gold atoms located approximately at $0, 0, 0$ and $0, \frac{1}{2}, \frac{5}{8}$ and two cadmium atoms located approximately at $\frac{1}{2}, 0, \frac{1}{2}$ and $\frac{1}{2}, \frac{1}{2}, \frac{1}{8}$. Since the exact positions of these atoms in the unit cell are not known, it is reasonable, for purposes of simplification, to describe the orthorhombic cell as face-centered with two gold atoms located approximately at $0, 0, 0$ and $0, \frac{1}{2}, \frac{1}{2}$ and two cadmium atoms located approximately at $\frac{1}{2}, 0, \frac{1}{2}$ and $\frac{1}{2}, \frac{1}{2}, 0$. The co-ordinates of an atom in β' referred to axes β' are then of the form

$$(\tfrac{1}{2}m_1 a,\ \tfrac{1}{2}m_2 b,\ \tfrac{1}{2}m_3 c),$$

where m_1, m_2, m_3 are integers and $(m_1+m_2+m_3)$ is even. The sites with m_1 even belong to gold atoms, and those with m_1 odd to cadmium atoms.

We shall now consider the atomic displacements involved in generating the β' structure from the β_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 β_1. Let the co-ordinate numbers of the four atoms defining a primitive unit cell of β_1 be:

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

where $(0,0,0)_{\beta_1}$ and $(0,1,0)_{\beta_1}$ are gold atoms and $(\frac{1}{2},\frac{1}{2},\frac{1}{2})_{\beta_1}$, $(\frac{1}{2},\frac{1}{2},-\frac{1}{2})_{\beta_1}$ are cadmium atoms. Following the method adopted by Jaswon & Wheeler (1948), and assuming that, of the many possible distortions of a primitive unit cell of β_1 by which the β' 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 β_1—β' transformation as being:

$$\left.\begin{array}{lll}(0,0,0)_{\beta_1} & \rightarrow (0,0,0)_{\beta'} & \text{Au atom,}\\ (0,1,0)_{\beta_1} & \rightarrow (0,\tfrac{1}{2},\tfrac{1}{2})_{\beta'} & \text{Au atom,}\\ (\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})_{\beta_1} & \rightarrow (\tfrac{1}{2},0,\tfrac{1}{2})_{\beta'} & \text{Cd atom,}\\ (\tfrac{1}{2},\tfrac{1}{2},-\tfrac{1}{2})_{\beta_1} & \rightarrow (\tfrac{1}{2},\tfrac{1}{2},0)_{\beta'} & \text{Cd atom.}\end{array}\right\} \qquad (8)$$

The correspondence in equation (8) between the initial positions, referred to axes β_1, and the final positions, referred to axes β', of the four atoms defining a primitive unit cell can be expressed alternatively by a linear relation of the type:

$$\begin{pmatrix}h'\\k'\\l'\end{pmatrix}_{\beta'} = (\tau)\begin{pmatrix}h\\k\\l\end{pmatrix}_{\beta_1}, \quad \tau = \frac{1}{2}\begin{pmatrix}2 & 0 & 0\\0 & 1 & -1\\0 & 1 & 1\end{pmatrix}, \qquad (9)$$

where (τ) is the matrix of a relation which involves change of axis, change of lattice parameter, and transformation displacement. The relation given in (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 (τ) is in fact the direction transformation matrix from β_1 to β'. Thus we have:

$$\begin{bmatrix}h'\\k'\\l'\end{bmatrix}_{\beta'} \rightleftharpoons \frac{1}{2}\begin{pmatrix}2 & 0 & 0\\0 & 1 & -1\\0 & 1 & 1\end{pmatrix}\begin{bmatrix}h\\k\\l\end{bmatrix}_{\beta_1}, \qquad (10)$$

and, using the inverse matrix, we have

$$\begin{bmatrix}h\\k\\l\end{bmatrix}_{\beta_1} \rightleftharpoons \begin{pmatrix}1 & 0 & 0\\0 & 1 & 1\\0 & -1 & 1\end{pmatrix}\begin{bmatrix}h'\\k'\\l'\end{bmatrix}_{\beta'}, \qquad (11)$$

where $[h',k',l']_{\beta'}$ are the indices of a given direction of β' transformed from the direction $[h,k,l]_{\beta_1}$ of β_1, and vice versa.

A similar operation yields the following plane transformation matrices:

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

$$\begin{pmatrix}h\\k\\l\end{pmatrix}_{\beta_1} \rightleftharpoons \frac{1}{2}\begin{pmatrix}2 & 0 & 0\\0 & 1 & 1\\0 & -1 & 1\end{pmatrix}\begin{pmatrix}h'\\k'\\l'\end{pmatrix}_{\beta'}, \qquad (13)$$

where $(h', k', l')_{\beta'}$ are the indices of a given plane of β' transformed from the $(h,k,l)_{\beta_1}$ plane of β_1, and vice versa.

4. Crystallographic mechanism of the β_1—β' 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 β_1 to β', or vice versa. The actual crystallographic mechanism of the β_1-β' 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 (Chang & Read, 1950) 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, β_1 and β'.

(*b*) The transformation takes place in a well-grown and annealed β_1 single crystal by the formation of a β' 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 β' to β_1, the opposite happens.

(*c*) An optically flat surface of the β_1 crystal transforms into an optically flat surface of the β' 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 β_1, and on the other side of the interface there is a single crystal of β' transformed from β_1.

(*e*) The slow-moving interface has been previously identified (Chang & Read, 1950) to be a (331)-type plane of the β_1 phase. The interface moves on transformation at a velocity (about 0·01 to 0·1 mm.sec.$^{-1}$) almost directly proportional to the rate of cooling (or heating) of the specimen.

Single crystals of β_1 with two flat surfaces across the length of the specimen were therefore prepared. The interface between β_1 and β' was maintained near the middle of the specimen. The two flat surfaces of β_1, A and B, transform, respectively, to two flat surfaces, A' and B', of β'. 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-

Table 2. *Determination of crystallographic mechanism of β_1—β' transformation*

	$(A'-A)$	$(B'-B)$
Crystal no. 2:		
Horizontal circle	$-67\pm2'$	$-18\pm2'$
Vertical circle	$-20\pm1'$	$-15\pm1'$

Shear plane $(\bar{3}31)_{\beta_1}$; shear direction $[323]_{\beta_1}$; degree of shear $\gamma_0 = 3°\ 2'$ ($\tan\gamma_0 = 0{\cdot}053$).

Crystal no. 7:		
Horizontal circle	$+33\pm1'$	$+55\pm1'$
vertical circle	$-40\pm1'$	$-89\pm2'$

Shear plane $(\bar{3}31)_{\beta_1}$; shear direction $[323]_{\beta_1}$; degree of shear $\gamma_0 = 2°\ 45'$ ($\tan\gamma_0 = 0{\cdot}047$).

circle optical goniometer accurate to within 2–3′. 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 & Troiano (1949). The results of two separate determinations are shown in Table 2.

The experimentally measured crystallographic mechanism of β_1—β' transformation is therefore a simple homogeneous shear of the type $(\bar{3}31)_{\beta_1}[323]_{\beta_1}$ by about 3°.

5. 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 (Table 1) as follows:

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

On the other hand, knowing the shear mechanism, we can calculate the displacements of the lattice point $(\alpha, \sqrt{2}\alpha, \sqrt{2}\alpha)$, i.e. U', V' and W', independently, without the knowledge of the lattice parameters of the β' phase. In other words, if U', V' and W' are known, we can calculate a, b and c according to (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,

X axis $[7.12.\overline{15}]_{\beta_1}$,

Y axis $[3.2.3]_{\beta_1}$,

Z axis $[\bar{3}.3.1]_{\beta_1}$.

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

$$\left.\begin{aligned} &\frac{\partial u}{\partial x}=0, \quad \frac{\partial u}{\partial y}=0, \quad \frac{\partial u}{\partial z}=0, \\ &\frac{\partial v}{\partial x}=0, \quad \frac{\partial v}{\partial y}=0, \quad \frac{\partial v}{\partial z}=\tan\gamma_0=0{\cdot}050, \\ &\frac{\partial w}{\partial x}=0, \quad \frac{\partial w}{\partial y}=0, \quad \frac{\partial w}{\partial z}=0, \end{aligned}\right\} \tag{15}$$

or

$$\left.\begin{aligned} &e_{xx}=\frac{\partial u}{\partial x}=0, \quad e_{yz}=\frac{\partial w}{\partial y}+\frac{\partial v}{\partial z}=0{\cdot}050, \\ &\qquad\qquad\qquad\qquad w_x=\frac{1}{2}\left(\frac{\partial w}{\partial y}-\frac{\partial v}{\partial z}\right)=-0{\cdot}025, \\ &e_{yy}=\frac{\partial v}{\partial y}=0, \quad e_{zx}=\frac{\partial u}{\partial z}+\frac{\partial w}{\partial x}=0, \quad w_y=\frac{1}{2}\left(\frac{\partial u}{\partial z}-\frac{\partial w}{\partial x}\right)=0, \\ &e_{zz}=\frac{\partial w}{\partial z}=0, \quad e_{xy}=\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}=0, \quad w_z=\frac{1}{2}\left(\frac{\partial v}{\partial x}-\frac{\partial u}{\partial y}\right)=0. \end{aligned}\right\} \tag{16}$$

Now we shall transform the strain components from reference axes X, Y, Z to other reference axes X', Y', Z', where

$$X'=[100]_{\beta_1}, \quad Y'=[01\bar{1}]_{\beta_1}, \quad Z'=[011]_{\beta_1}$$

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:

$$\left.\begin{array}{cccc} & X & Y & Z \\ & [7.12.\overline{15}] & [3.2.3] & [\bar{3}.3.1] \\ X'[100] & l_1=\dfrac{7}{\sqrt{(418)}} & m_1=\dfrac{3}{\sqrt{(22)}} & n_1=-\dfrac{3}{\sqrt{(19)}}, \\ Y'[01\bar{1}] & l_2=\dfrac{27}{\sqrt{(836)}} & m_2=-\dfrac{1}{\sqrt{(44)}} & n_2=\dfrac{2}{\sqrt{(38)}}, \\ Z'[011] & l_3=-\dfrac{3}{\sqrt{(836)}} & m_3=\dfrac{5}{\sqrt{(44)}} & n_3=\dfrac{4}{\sqrt{(38)}}. \end{array}\right\} \tag{17}$$

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

$$\left.\begin{aligned} e_{x'x'} &= l_1^2 e_{xx}+m_1^2 e_{yy}+n_1^2 e_{zz}+m_1 n_1 e_{yz} \\ &\qquad +n_1 l_1 e_{zx}+l_1 m_1 e_{xy}, \\ e_{y'z'} &= 2l_2 l_3 e_{xx}+2m_2 m_3 e_{yy}+2n_2 n_3 e_{zz} \\ &\qquad +(m_2 n_3+m_3 n_2)\,e_{yz}+(n_2 l_3+n_3 l_2)\,e_{zx} \\ &\qquad +(l_2 m_3+l_3 m_2)\,e_{xy}, \\ w_{x'} &= l_1 w_x+m_1 w_y+n_1 w_z. \end{aligned}\right\} \tag{18}$$

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:

$$\left.\begin{aligned} U' &= e_{x'x'}X'+\tfrac{1}{2}e_{x'y'}Y'+\tfrac{1}{2}e_{z'x'}Z'-w_{z'}Y'+w_{y'}Z', \\ V' &= \tfrac{1}{2}e_{x'y'}X'+e_{y'y'}Y'+\tfrac{1}{2}e_{y'z'}Z'-w_{x'}Z'+w_{z'}X', \\ W' &= \tfrac{1}{2}e_{z'x'}X'+\tfrac{1}{2}e_{y'z'}Y'+e_{z'z'}Z'-w_{y'}X'+w_{x'}Y'. \end{aligned}\right\} \tag{19}$$

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

$$U'=-0{\cdot}0514\alpha, \quad V'=+0{\cdot}0242\alpha \quad W'=+0{\cdot}0485\alpha. \tag{20}$$

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

$$a = 3{\cdot}1460, \quad b = 4{\cdot}7704, \quad c = 4{\cdot}8510\,\text{kX}.$$

The correspondence between the calculated and measured (X-ray) 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. along the b axis of the orthorhombic cell will bring almost exact agreement between the calculated and measured lattice parameters of the orthorhombic phase.

This work was done under contract AT(30–1)–904 of the Atomic Energy Commission, United States of America. The author is obliged to the Commission for the permission to publish the paper. He also acknowledges with thanks the helpful suggestions of Dr T. A. Read, Columbia University, during the course of the work.

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Acta Cryst. (1951). **4**, 324

The Crystal Structure of Lauric Acid

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(*Received* 9 *November* 1950)

Lauric acid (form C or α), $C_{12}H_{24}O_2$, is monoclinic with $a = 9{\cdot}524$, $b = 4{\cdot}965$, $c = 35{\cdot}39$ A., $\beta = 129°\ 13'$. The cell contains four molecules; density observed 1·032, calculated 1·034 g.cm.$^{-3}$. The space group is C^5_{2h}–$P2_1/a$. Fourier projections were prepared and atomic co-ordinates determined. The angle of tilt $\tau = 54°\ 52'$.

Introduction

Lauric acid is known to exhibit polymorphism. Crystals of very pure lauric acid, prepared in these laboratories, were grown from ethanol solution. They proved to be in the form C of Francis & Piper (1939) or form α of Thibaud & Duprè de la Tour (1930a, b, 1932) with melting-point of 44·8° C. and setting-point 43·9° C.

Determination of X-ray data

The following data were determined from moving-film zero- and n-layer Weissenberg photographs about the a and b axes and powder photographs using Ni-filtered Cu $K\alpha$ radiation:

Molecular formula $C_{12}H_{24}O_2$.
Molecular weight = 200·31.
The crystal is monoclinic with

$$a = 9{\cdot}524 \pm 0{\cdot}02,$$
$$b = 4{\cdot}965 \pm 0{\cdot}01,$$
$$c = 35{\cdot}39 \pm 0{\cdot}07\ \text{A.},$$
$$\beta = 129°\ 13' \pm 1',$$
$$c \sin\beta = 27{\cdot}42 \pm 0{\cdot}06\ \text{A.}$$

Four molecules per unit cell.
Density calc. = 1·034, density meas. = 1·032 g.cm.$^{-3}$.
Absent reflexions: $(h0l)$ when h odd, $(0k0)$ when k odd.
Space group: C^5_{2h}–$P2_1/a$.

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