Acta Cryst. (1950). **3**, 479

Mechanical twinning in white tin.

By R. Clark, G. B. Craig and B. Chalmers, *Department of Metallurgical Engineering, University of Toronto, Toronto 5, Canada*

Introduction

The twinning plane in white tin has been variously reported as {331} (Schmid & Boas, 1935; Barrett, 1943; Elam, 1935) and also as {301} (Chalmers, 1935). The present investigation was undertaken to ascertain the reason for this discrepancy.

Experimental procedure

Chemically pure tin (99·987 % Sn) was used to grow single crystals by means of the technique of Chalmers (1940). The orientation of the specimens was controlled in order to have conditions favourable for twinning by impact and by stretching. (An orientation suitable for twinning by impact is not suitable for twinning in tension.) Twins were produced by impact (Chalmers, 1935) in two specimens, and by stretching in one other crystal. The crystallographic relationship between the parent crystal and the twin bands was determined from back-reflexion Laue photographs analysed by means of a technique described by Greninger (1935). Fig. 1 shows the points of incidence (*A* and *B*) of the X-ray beam, which was normal to the axis of a specimen twinned by impact.

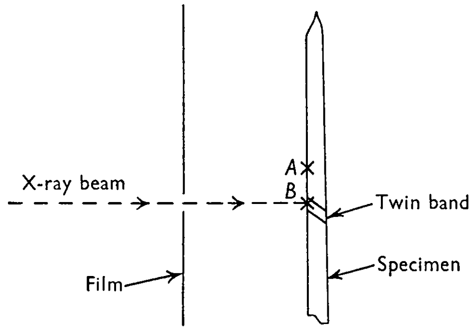
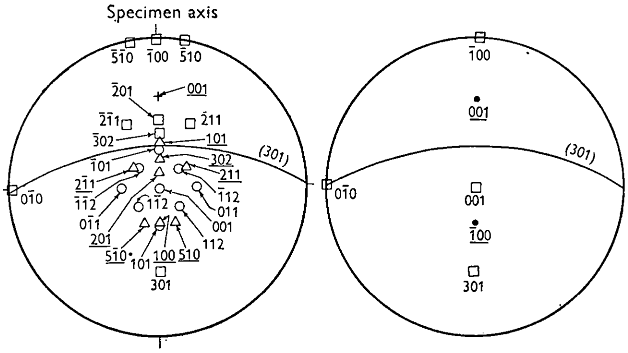


Fig. 1. X-ray geometry.



(*a*) (*b*)

Fig. 2. Stereographic projections showing (*a*) the relative orientation of the twinned crystal section, and (*b*) a twinned crystal orientation derived from reflexion of the standard projection across a (301) plane. Symbols: (*a*) △ observed poles of twin band; + pole of twin band calculated from observed poles; ○ observed poles of parent crystal; □ poles of parent crystal calculated from observed poles. (*b*) □ poles of standard 001 projection; • poles of (301) twin orientation.

The stereographic projection in Fig. 2(*a*) shows the crystallographic relationship between the twinned and untwinned crystals, the orientation of the latter being nearly identical with that of a standard (001) projection of body-centred tetragonal tin with $a = 5{\cdot}8194$ and $c = 3{\cdot}1753$ A. (Barrett, 1943). It can be seen that the equivalent planes are mirror images in a (301) plane. Fig. 2(*b*) shows the (301) twin orientation of a standard (001) projection which agrees with the experimental evidence given in Fig. 2(*a*).

Discussion

The X-ray investigation substantiated the results of Chalmers (1935). However, examination of the work of Mügge (1917, 1927) and of Tanaka & Kamio (1931) revealed how the discrepancy between {331} and {301} twinning arose.

Tanaka & Kamio considered a tetragonal diamond-like structure with cell dimensions $a = 8{\cdot}22$ and $c = 3{\cdot}17$ A. (van Arkel, 1924). The same disposition of atoms can, however, be referred to a smaller body-centred tetragonal cell with $a = 5{\cdot}8194$ and $c = 3{\cdot}1753$ A. (Barrett, 1943). This means that there has not been any change in the relative position of the atoms, but simply a different choice of axes. It is therefore concluded that the discrepancy between the two twin planes arose with the acceptance of the body-centred tetragonal lattice without revision of the Miller indices of the twinning plane.

References

Arkel, A. E. van (1924). *Proc. Acad. Sci. Amst.* **27**, 97.

Barrett, C. S. (1943). *Structure of Metals.* New York: McGraw-Hill.

Chalmers, B. (1935). *Proc. Phys. Soc. Lond.* **47**, 733.

Chalmers, B. (1940). *Proc. Roy. Soc.* A, **175**, 100.

Elam, C. E. (1935). *Distortion of Metal Crystals.* Oxford: Clarendon Press.

Greninger, A. B. (1935). *Trans. Amer. Inst. Min. (Metall.) Engrs*, **117**, 61.

Mügge, O. (1917). *Zbl. Min. Geol. Paläont.* p. 233.

Mügge, O. (1927). *Z. Krystallogr.* **65**, 603.

Schmid, E. & Boas, W. (1935). *Kristallplastizität.* Berlin: Springer.

Tanaka, K. & Kamio, K. (1931). *Mem. Coll. Sci. Kyoto*, A, **14**, 79.

Acta Cryst. (1950). **3**, 479

An exception to Friedel's law in electron diffraction. II. Theoretical consideration.

By Kazutake Kohra, *Department of Applied Physics, Faculty of Engineering, Kyushu University, Fukuoka, Japan,* Ryozi Uyeda, *Physical Institute, Nagoya University, Nagoya, Japan* and Shizuo Miyake, *Tokyo Institute of Technology, Oh-Okayama, Meguro-ku, Japan*

(*Received* 20 *February* 1950)

In the previous note, Miyake & Uyeda (1950) reported an observation that Friedel's law ceases to hold in electron diffraction by the cleavage face (110) of zincblende: the intensities of (*hhk*) and $(hh\bar{k})$ reflexions are not equal when they are excited simultaneously by the primary electron beam directed in the [1$\bar{1}$0] azimuth (Fig. 1). In the present note, we interpret this phenomenon from the standpoint of the dynamical theory of diffraction adopting the general procedure of Bethe (1928).

Let us assume, according to the experimental condition, that the amplitudes ψ_0, ψ_l and ψ_m of the primary and two diffracted waves within the crystal are large compared with those of the other waves, then we have the reduced fundamental equations

$$\left.\begin{aligned}(\varkappa^2-k_0^2)\,\psi_0+v_{-l}\psi_l+v_{-m}\psi_m&=0,\\ v_l\psi_0+(\varkappa^2-k_l^2)\,\psi_l+v_{l-m}\psi_m&=0,\\ v_m\psi_0+v_{m-l}\psi_l+(\varkappa^2-k_m^2)\,\psi_m&=0,\end{aligned}\right\}\qquad(1)$$

where $\varkappa^2=K^2+v_0$, and $\mathfrak{k}_g=\mathfrak{k}_0+2\pi\mathfrak{g}$ in general. The symbols used here are the same as those adopted by Bethe, and l and m stand for (hhk) and $(hh\bar{k})$ respectively. The Fourier coefficients v_i's are complex and conjugate to v_{-i}'s in general as the zincblende crystal has no centre of symmetry; v_l is also conjugate to v_m if the origin of the co-ordinate is taken on a mirror plane parallel to (110).

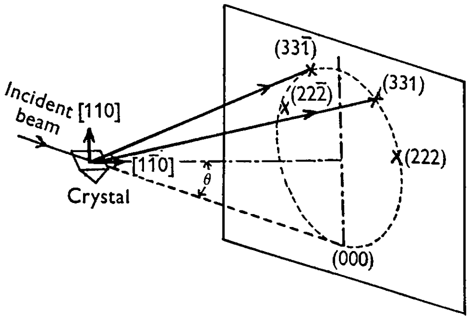


Fig. 1. Geometry of the phenomenon.

The secular equation of (1) determines the dispersion surface, and, if the boundary conditions are given, six wave points are fixed on it, but we are concerned with only three of them as usual, and denote them by $j=1, 2$ and 3 respectively. Then the amplitudes of the diffracted waves turn out to be

$$\psi_{lj}=\frac{v_{l-m}v_m-v_lQ_j}{Q_j^2-|v_{l-m}|^2}\,\psi_{0j},\quad \psi_{mj}=\frac{v_{m-l}v_l-v_mQ_j}{Q_j^2-|v_{l-m}|^2}\,\psi_{0j},\qquad(2)$$

where $Q_j\equiv\varkappa^2-k_{lj}^2=\varkappa^2-k_{mj}^2$. In the present case, being a 'Bragg case', two of the wave points, say $j=1$ and 2, become imaginary in a certain region of the glancing angle θ (Fig. 1). Outside this region $\mathfrak{k}_{lj}$ (or $\mathfrak{k}_{mj}$) are real for $j=1$, 2 and 3, while inside it the components of $\mathfrak{k}_{l1}$ and $\mathfrak{k}_{l2}$ normal to the boundary surface are complex and conjugate to each other and $\mathfrak{k}_{l3}$ is real. In the former region $|\psi_{lj}|=|\psi_{mj}|$ holds for all j's, so that the intensity of the two diffracted waves are always equal to each other, and no asymmetry in intensity should occur. This situation also applies to the 'Laue case' generally. In the latter region, on the other hand, corresponding to that of selective reflexion, $|\psi_{lj}|\neq|\psi_{mj}|$ in general, and asymmetry may result. In this region $\mathfrak{k}_{l1}$, say, gives a damped wave and $\mathfrak{k}_{l2}$ an enhanced one within the crystal, and the amplitude of the latter wave must vanish if the crystal extends to semi-infinity. We accordingly obtain approximately the following relations between the amplitudes Ψ_0, Ψ_l and Ψ_m of the incident and diffracted wave in vacuum:

$$\left.\begin{aligned}\Psi_l&=\frac{\Gamma_0(\Gamma_l+\gamma_{l1})}{\Gamma_l(\Gamma_0+\gamma_{01})}\times\frac{v_{l-m}v_m-v_lQ_1}{Q_1^2-|v_{l-m}|^2}\,\Psi_0,\\ \Psi_m&=\frac{\Gamma_0(\Gamma_m+\gamma_{m1})}{\Gamma_m(\Gamma_0+\gamma_{01})}\times\frac{v_{m-l}v_l-v_mQ_1}{Q_1^2-|v_{l-m}|^2}\,\Psi_0,\end{aligned}\right\}\qquad(3)$$

where Γ_0, Γ_l, Γ_m; γ_{01}, γ_{l1} and γ_{m1} mean respectively the magnitudes of the normal components of the wave vectors $\mathfrak{K}_0$, $\mathfrak{K}_l$, $\mathfrak{K}_m$; $\mathfrak{k}_{01}$, $\mathfrak{k}_{l1}$ and $\mathfrak{k}_{m1}$. In the present case $\Gamma_l=\Gamma_m$ and $\gamma_{l1}=\gamma_{m1}$. Denote the powers of the incident and two diffracted rays by P_0, P_l and P_m respectively, then the latter two are found to be

$$P_l=\frac{\Gamma_l}{\Gamma_0}\frac{|\Psi_l|^2}{|\Psi_0|^2}P_0,\quad P_m=\frac{\Gamma_m}{\Gamma_0}\frac{|\Psi_m|^2}{|\Psi_0|^2}P_0.\qquad(4)$$

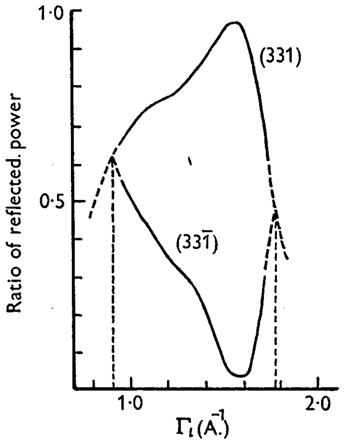


Fig. 2. Ratios of reflected power. The vertical broken lines correspond to the selective range of reflexion, for which alone our numerical calculation is performed. The fact that the sum of the two ratios exceeds unity is due to the approximation of the calculation.

From (3) and (4), the difference in the reflexion powers is obtained as

$$P_l-P_m=\frac{4\Gamma_0\,|\Gamma_0+\gamma_{01}|^2P_0}{\Gamma_l\,|\Gamma_l+\gamma_{l1}|^2\,|Q_1^2-|v_{l-m}|^2|^2}\times I(Q_1)\,I(v_mv_{-l}v_{l-m}),\qquad(5)$$

where $I(\ )$ means the value of the imaginary part of the expression in the bracket. The right-hand side of (5) is of course independent of the choice of the origin of the coordinates and also of the position of the boundary surface as long as it is parallel to (110). As $I(Q)$ is not zero in the region of the selective reflexion, an asymmetry should occur when $I(v_mv_{-l}v_{l-m})$ is not zero. The latter condition is fulfilled for zincblende and the expected asymmetry of intensity is actually observed in our experiment.

We carried out a numerical calculation for the simultaneous reflexion of (331) and (33$\bar{1}$), on which the most remarkable asymmetry was observed (Miyake & Uyeda, 1950, Fig. 4). The values of v_i's are computed by using Pauling–Sherman's f-value corrected with the Debye–Waller factor. We have $v_l=v_m^*=v_{-m}=v_{-l}^*=0{\cdot}58-0{\cdot}33i$ and $v_{l-m}=v_{m-l}=0{\cdot}64$. The result of the calculation (Fig. 2) shows that (331) has a single large peak, while (33$\bar{1}$) splits into two small peaks. This feature is in general accordance with the observations of Miyake & Uyeda.

Though the dynamical effect of 'weak rays' within the crystal is wholly neglected in the above theory for the sake of simplicity, we also confirmed that their inclusion by the procedure of Bethe (1928) does not change the general feature of the results. It must, however, be remembered that the (222) and (22$\bar{2}$) reflexions become of considerable importance when the conditions for the (331) and (33$\bar{1}$) reflexions are fulfilled simultaneously, so that it is not adequate to assume the former as weak rays. Their effect may be responsible for the more complicated intensity distribution as compared with that observed and the one shown in Fig. 2.

At any rate we believe that the observation on the apparent violation of Friedel's law in electron diffraction can reasonably be explained as a special case of the well-known phenomenon of *Aufhellung*. The effect is to be expected only in the 'Bragg case' and never in the 'Laue case'. A similar effect may be expected to occur in the case of X-ray diffraction by a polar crystal.

References

Bethe, H. (1928). *Ann. Phys., Lpz.*, **87**, 55.
Miyake, S. & Uyeda, R. (1950). *Acta Cryst.* **3**, 314.

Acta Cryst. (1950). **3**, 481

International Union of Crystallography

Second General Assembly and International Congress, Stockholm, 27 June–3 July 1951

By kind invitation of the Swedish National Committee for Crystallography the Second General Assembly and International Congress of the Union will be held in Stockholm from 27 June to 3 July 1951. A Local Committee has been established under the Chairmanship of A. Westgren, Vice-President of the Union, with F. E. Wickman as Secretary.

Membership

Delegates to the General Assembly, which will be concerned with the formal business of the Union, will be nominated by the National Committees. Crystallographers throughout the world are, however, cordially invited to attend the International Congress; it is particularly hoped that they will assist the Union by bringing the Congress to the notice of their colleagues, by press announcements and otherwise, so that the attendance may be large and fully representative of crystallographic research in all countries. The Union is unfortunately not in a position to provide funds to assist delegates in meeting travelling expenses.

A grant towards the expenses of the Congress has been generously made by the Swedish Government. It is, however, a condition of the grant that delegates shall themselves make some contribution. All those attending will, therefore, be required to pay a membership fee of 50 Swedish crowns.

Programme

The subjects selected for consideration are:

1. Instruments and Measurements.
2. New Developments in Structure Determination.
3. Mineral Structures.
4. Metal Structures.
5. Inorganic Structures.
6. Organic Structures.
7. Proteins and Related Structures.
8. Random and Deformed Structures.
9. Thermal Transformations.
10. Crystal Growth.
11. Neutron Diffraction.
12. Miscellaneous.

The Executive Committee has decided that no report of the Congress shall be published, it being felt that most of the contributions will find their way into the scientific literature in the normal manner and that the expense of separate publication would not be warranted. Full abstracts of the contributions will, however, be distributed in advance; speakers will then be expected to present their papers quite briefly at the Congress in order that ample time may be available for discussion.

Exhibition

It has unfortunately not been found practicable to arrange any exhibition of instruments or equipment in connexion with the Congress. It is possible, however, that a number of instrument manufacturers represented in Stockholm will take the opportunity of themselves arranging small exhibits of crystallographic interest.

Excursions

Arrangements have been made for a visit to Uppsala University and will probably also be made for visits to localities of mineralogical interest. Details will be announced later.

It is hoped also to arrange a programme of excursions and other events for the benefit of friends accompanying those attending the Congress.

Symposia

It is proposed to hold two Symposia on the following topics:

1. Advanced Techniques in Structure Determination.
2. Electron Diffraction in Liquids and Gases.

These Symposia are intended primarily for specialist workers in these fields, but in so far as accommodation is available all crystallographers will be welcome. The Symposia will probably be held on the days immediately following the Congress but one or more sessions may also be arranged during the period 27 June–3 July.

Languages

Although contributions may be presented in any language, the Executive Committee feels that those in English, French and German, and especially those in English, will be most readily understood by the majority of the