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ELECTRON DIFFRACTION FROM PERIODIC ARRANGEMENTS OF STACKING FAULTS:
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ELECTRON DIFFRACTION FROM PERIODIC ARRANGEMENTS OF STACKING FAULTS:
APPLICATION TO ANTI-PHASE DOMAIN BOUNDARIES IN ORDERED COPPER-GOLD (Cu Au) ALLOY

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ABSTRACT

The nature of the transmission electron diffraction pattern from Cu Au II alloy films has been studied in detail. The interpretations given by earlier workers have been shown to be incomplete. In the present paper, the form of the electron diffraction pattern from a crystal with a periodic arrangement of stacking faults has been calculated, taking account of Fraunhofer effects at plane faults. The results of this calculation have been applied to the periodic anti-phase domain boundaries in the Cu Au I structure which define the Cu Au II structure. The calculated intensity distributions about the direct spot and Bragg spots agree with experimental observation. Contributions to the intense satellite spots about the direct spot which cannot be explained by kinematical theory are predicted by this model.
I. INTRODUCTION

The selected area diffraction patterns from an area of a crystal containing a stacking fault have been explained by Whelan and Hirsch\(^1\) and Fitzgerald and Mannami.\(^2\) Whelan and Hirsch have explained the satellite spots observed on either side of the Bragg spot in electron diffraction patterns from a stacking faulted crystal by transferring the dynamical construction for a stacking fault on the dispersion surface to the reflecting sphere. Fitzgerald and Mannami have shown that the spikes and subsidiary peaks in the intensity distribution about the Bragg spots can be described as a Fraunhofer diffraction effect from stacking faults. The wave function of an electron passing through a stacking fault to form the Bragg spot is different from that of an electron passing through the perfect region surrounding the stacking fault. The waves giving rise to the spikes have a non-zero value only along the path of an electron passing through the stacking fault. These differences in wave function give a Fraunhofer diffraction pattern similar to that of a slit.

In the present paper the form of electron diffraction patterns from a periodic arrangement of stacking faults is calculated and the results are used to explain some features of electron diffraction patterns from the periodic arrangement of antiphase domain boundaries in the ordered alloy Cu Au II.
II. FRAUNHOFER DIFFRACTION FROM A PERIODIC ARRANGEMENT OF STACKING FAULTS

Whelan and Hirsch\(^1\) have shown that for an incident electron wave, \(\psi_I \exp (2\pi i K \cdot r)\), neglecting inelastic scattering, the wave function of the electron in a crystal containing a stacking fault (shown diagrammatically in Fig. 1) may be expressed as

\[
\phi(r) = \sum_{i=1}^{2} \sum_{h=0,g} \phi_i^{(i)} \exp(2\pi i k_i^{(i)} \cdot r) + \sum_{i=1}^{2} \sum_{h=0,g} \phi_i'^{(i)} \exp(2\pi i k_i'^{(i)} \cdot r)
\]

This is the two beam approximation, \(g\) is the reciprocal lattice vector of the excited Bragg reflection,

\[
k_o^{(i)} = D^{(i)}_0, \quad k_g^{(i)} = D^{(i)} G,
\]

\[
k_o^{(i)'} = D^{(i)}_0 \quad \text{and} \quad k_g^{(i)'} = D^{(i)'} G.
\]

The relation of these vectors to the incident wave vector \(K\) are shown in Fig. 2. The wave amplitudes \(\phi_i^{(i)}\) (\(h=0,g\)) are zero outside of the shaded region in Fig. 1. The wave function on the exit surface, points on which are represented by the position vector \(R_e(X,Y)\), is
$$\phi(R_e) \begin{cases} = \sum_{i,h} \phi_{h}^{(i)}(R_e) \exp(2\pi k_{h}^{(i)} \cdot R_e) + \sum_{i,h} \phi_{h}^{(i)'}(R_e) \exp(2\pi k_{h}^{(i)'} \cdot R_e) \quad \text{(on S)} \quad (2a) \\ = \sum_{i,h} \phi_{h}^{(i)} \exp(2\pi k_{h}^{(i)} \cdot R_e) \quad \text{(outside S),} \quad (2b) \end{cases}$$

where \( S \) is the projected area of the stacking fault parallel to \( K \) on the exit surface. \( \phi_{h}^{(i)}(R_e) \) and \( \phi_{h}^{(i)'}(R_e) \) are functions of \( x, x^{(1)}, x^{(2)} \) (parameters expressing the condition of diffraction at wave points \( D^{(1)} \) (and \( D^{(2)} \), \( D^{(1)'} \) and \( D^{(2)'} \) respectively on the dispersion surface in Fig. 2), \( \alpha \) (the phase shift of the electron wave due to the stacking fault), \( \delta \) (the angle between the normal to the crystal surface \( n_e \) and the normal to the stacking fault plane \( n_s \) and \( R_e \)). For details of the evaluation of \( \phi_{h}^{(i)}(R_e) \) and \( \phi_{h}^{(i)'}(R_e) \) in terms of these parameters, see the appendix to reference 2.

According to Kirchoff's theory of diffraction in optics\(^3\) the Fraunhofer pattern \( F(q_x, q_y) \) is the Fourier transform of the amplitude \( \phi(X,Y) \) across the diffracting aperture and vice-versa, i.e.

$$F(q_x, q_y) = C \int \int \phi(X,Y) \exp(2\pi i(q_xX + q_yY)) \, dx \, dy \quad (3a)$$

$$\phi(X,Y) = C \int \int F(q_x, q_y) \exp(-2\pi i(q_xX + q_yY)) \, dq_x \, dq_y \quad (3b)$$

where \( C \) is a constant, \( q_x \) and \( q_y \) equal \( |k| \sin \theta_X \) and \( |k| \sin \theta_Y \) respectively and \( 90^\circ - \theta_X \) and \( 90^\circ - \theta_Y \) are the angles between the wave...
vector \( \mathbf{k} \) and the X and Y axes respectively. These relations can be applied to an electron wave.

For a periodic arrangement of \( N \) stacking faults contained within the select area diffraction aperture, Eq. (2a) represents the wave function over the projected area \( S_r \) of the \( r \)th stacking fault and Eq. (2b) represents the wave function over the area \( A_r \) (see Fig. 3). Since the diffracted wave amplitudes \( \phi_h^{(i)} \) and \( \phi_h^{(i)'} \) are proportional to \( V_h \), the Fourier coefficient of lattice potential, the phase shift of diffracted waves from the area \( S_r + A_r \) is \( \phi_r = 2\pi h \cdot R_r \) with respect to the reference area \( S_{-1} + A_{-1} \), and attention must be paid to phase differences when evaluating the Fourier transform from this array of stacking faults. \( R_r \) is the shift of \( S_r + A_r \) with respect to \( S_{-1} + A_{-1} \).

For \( N \) stacking faults Eq. (2) becomes

\[
\phi(\mathbf{R}_e) \begin{cases} 
= \sum_r \sum_i e^{i\phi_r} [\sum_h \phi_h^{(i)} (R_e) \exp(2\pi i k_h^{(i)'} R_e)] \\
+ \sum_i [\sum_h \phi_h^{(i)'} (R_e) \exp(2\pi i k_h^{(i)'} R_e)] \quad \text{(on all } S_r \text{)} \\
= \sum_r \sum_i e^{i\phi_r} [\sum_h \phi_h^{(i)} \exp(2\pi i k_h^{(i)} R_e)] \quad \text{(on all } A_r \text{)},
\end{cases}
\]

where \( h \) takes the values 0 and \( g \) and \( r \) takes the values from \(-N/2\) to \(+N/2\) excluding zero. For waves contributing to the intensity distribution about the direct spot (i.e. \( h = 0 \)), \( \phi_r = 0 \) always.

The Fourier transform of Eq. (3') is the summation of eight terms.
\[ F(q_x, q_y) = \sum_{i=1}^{4} f^{(i)}_o(q_x, q_y) + \sum_{i=1}^{4} f^{(i)}_g(q_x, q_y), \]  

where

\[ f^{(1)}_o(q) = \int_{\text{crystal surface}} (\sum_{i=1}^{2} \phi^{(i)}_o) \exp(2\pi i (K_t - q) \cdot R_e) \, d\tau_e, \]  

\[ f^{(2)}_o(q) = \sum_{r} \int_{S_r} [\sum_{i=1}^{2} \phi^{(i)}_o(R_e) - \phi^{(i)}] \exp(2\pi i (K_t - q) \cdot R_e) \, d\tau_e, \]

\[ f^{(3)}_o(q) = \sum_{r} \int_{S_r} (\phi^{(1)'}_o(R_e)) \exp(2\pi i (K_t + A^{(1)} - q) \cdot R_e) \, d\tau_e, \]

\[ f^{(4)}_o(q) = \sum_{r} \int_{S_r} (\phi^{(2)'}_o(R_e)) \exp(2\pi i (K_t + A^{(2)} - q) \cdot R_e) \, d\tau_e, \]

and for the diffracted waves with \( \alpha = 2\pi \mathbf{g} \cdot \mathbf{R} \neq 0 \)

\[ f^{(1)}_g(q) = \int_{\text{crystal surface}} (\sum_{i=1}^{2} \phi^{(i)}_g) \exp(2\pi i (K_t + g - q) \cdot R_e) \, d\tau_e, \]

\[ f^{(2)}_g(q) = \sum_{r} e^{i \phi_r} \int_{S_r} [\sum_{i=1}^{2} \phi^{(i)}_g(R_e) - \phi^{(i)}] \] 
\[ \times \exp(2\pi i (K_t + g - q) \cdot R_e) \, d\tau_e, \]

\[ f^{(3)}_g(q) = \sum_{r} e^{i \phi_r} \int_{S_r} (\phi^{(1)'}_g(R_e)) \exp(2\pi i (K_t + g + A^{(1)} - q) \cdot R_e) \, d\tau_e, \]
for \( f_h^{(3)} (q) \)

\[ Q_X = (K_t + h + \Delta^{(1)}) X \]

\[ - \Delta k_o \left( \sqrt{1 + x^2_{(1)}} - \sqrt{1 + x^2} \right) \tan \delta, \]

and for \( f_h^{(4)} (q) \)

\[ Q_X = (K_t + h + \Delta^{(2)}) X \]

\[ + \Delta k_o \left( \sqrt{1 + x^2_{(2)}} - \sqrt{1 + x^2} \right) \tan \delta, \]

where \( h \) takes the values of 0 and \( g \).

The intensity distribution around the direct spot \( (q = K_t) \) is proportional to

\[ \left| \sum_{i=1}^{4} f^{(i)} (q) \right|^2 \] (10)

because \( \sum_{i=1}^{4} f^{(i)} (q) \) is approximately zero when \( q \) is almost equal to \( K_t \). This intensity distribution has the following characteristics:

(a) Three principal maxima at

\[ q_X = (K_t) X \] (due to \( f^{(1)}_o (q) \) and \( f^{(2)}_o (q) \)),

\[ q_X = (K_t + \Delta^{(1)}) X - \Delta k_o \left( \sqrt{1 + x^2_{(1)}} - \sqrt{1 + x^2} \right) \tan \delta \]

(due to \( f^{(3)}_o (q) \))

and \( q_X = (K_t + \Delta^{(2)}) X + \Delta k_o \left( \sqrt{1 + x^2_{(2)}} - \sqrt{1 + x^2} \right) \tan \delta \)

(due to \( f^{(4)}_o (q) \)).
(b) Subsidiary maxima distributed symmetrically about each of these three principal maxima at distances \( n/\delta \) where \( n \) takes integral values. The peak height of each of these subsidiary maxima depends on the value of the factor

\[
\frac{\sin[\pi Z \cot \delta (Q-q)_X]}{[\pi Z \cot \delta (Q-q)_X]}
\]

The intensity distribution around a reciprocal lattice point \((q = K + g)\) is proportional to

\[
\left| \sum_{g} f_{(1)}^{(g)} (q) \right|^2.
\]

The nature of the intensity distribution in this case depends upon the value of \((\phi_{(n+1)} - \phi_{-(n+1)})\) in Eq. (9).
III. STRUCTURE OF CuAu II ALLOY

Copper gold alloy becomes ordered below a temperature of approximately 420°C to form CuAu I, a modified f.c.c. structure in which alternate (002) planes contain all copper and all gold atoms. The orthorhombic CuAu II phase is formed when the alloy is annealed just below the transition temperature for formation of CuAu I. The unit cell of the CuAu II structure is shown in Fig. 4 and contains ten cells of the f.c.c. type. Half way along the a_1 axis of the unit cell a phase change occurs; at this boundary the (002) planes containing all gold atoms oppose (002) planes containing all copper atoms. The structure, therefore, consists of domains with adjacent domains in antiphase.

This structure was first found by x-ray diffraction by Johansson and Linde^4 and has subsequently been investigated by transmission electron diffraction and microscopy by Ogawa and Watanabe,^5 Ogawa et al.,^6 Glossop and Pashley^7 and Fujima et al. The condition under which the contrast from these domain boundaries is visible in the electron microscope has been studied by Fisher and Marcinkovski.^9,10

The unit cell parameters in Fig. 4 are the same as those used by Glossop and Pashley to describe the CuAu II structure. The phase change which occurs half way along the orthorhombic CuAu II unit cell produces a lattice shift equal to a_2/2 + a_3/2. At this boundary there is a different arrangement of nearest neighbors compared with those in the interior of each domain. The spacing between the two planes adjacent to the boundary is slightly larger than the corresponding spacings away from the boundary. In Fig. 4, a_1', a_2', and a_3' are the lengths
of the sides of the approximate f.c.c. cell, \( a'_1 = a'_2 \) and \( a'_3 = 0.92a'_1 \).
For the orthorhombic cell \( a'_1 = 2(M + \delta)a'_1, a'_2 = a'_2 \) and \( a'_3 = a'_3 \). The
spacing between the two adjacent planes at the phase boundary is
given by \( a'_1/2 + \delta a'_1 \). \( M \) is normally equal to five in CuAu II, and \( \delta \)
is equal to 0.015. This value of \( \delta \) was detected by Johansson and Linde.
IV. ELECTRON DIFFRACTION FROM CuAu II ALLOY

Electron diffraction patterns from CuAu II alloy films have been studied in detail by Ogawa and co-workers and by Glossop and Pashley. The electron diffraction pattern obtained when the electron beam is directed along the [001] axis is shown in Fig. 5. The direct spot has a group of satellite spots situated symmetrically on either side. Each satellite spot is at a distance n/d from the direct spot where n is an integer and d = 2 x 10^{-7} cm is the spacing between anti-phase domain boundaries. The intensity of the satellite spots decreases with distance from the centre spot and the third order spot is usually very faint. A similar distribution of satellite spots is observed about the normal reflections (i.e. (200) and (220) in the CuAu I structure). The superlattice spots such as (110) in the CuAu I lattice split into satellites spaced apart by a distance l/d and arranged symmetrically about the normal position of this superlattice reflection before periodic ordering of anti-phase boundaries occurs.

The intensity distribution about superlattice spots in the electron diffraction patterns from CuAu II is adequately explained by kinematical theory as shown by Ogawa and Watanabe^5 and Glossop and Pashley.^7 However, the strength of the intensity distributions about both the direct spot and the normal diffraction spots cannot be explained by kinematical arguments. In fact, for δ = 0 the satellites around the direct spot are forbidden as shown by Glossop and Pashley. For δ = 0.015, the value obtained by Johansson and Linde, Glossop and Pashley found that the intensity of the first satellite at the split super-
lattice spots B (Fig. 6) should be 280 times stronger than the first satellite at the direct spot A. In practice, the direct spot satellite has a greater intensity than this superlattice satellite. Glossop and Pashley attempted to explain this intensity anomaly about the direct spot by suggesting that multiple scattering effects contribute to the intensity of satellite spots about the direct spot. Ogawa and co-workers have suggested that the enhanced intensity is due to some type of lattice or structure factor modulation. Both effects probably contribute to the satellite intensities about the direct spots. However, Fraunhofer effects at anti-phase boundaries must also be considered since, even for a single stacking fault, intense maxima can be observed close to Bragg spots and the direct spot in electron diffraction patterns.2
V. CALCULATION OF FRAUNHOFER EFFECTS IN ELECTRON DIFFRACTION PATTERNS FROM CuAu II ALLOYS

For a periodic arrangement of anti-phase domain boundaries, the intensity distribution due to Fraunhofer effects about the direct spot is given by expression (10). The interference functions for superlattice reflections take the form given by (9) where

$$\frac{\phi(n+1) - \phi(n+1)}{2} = \pi/2.$$

Therefore, for superlattice reflections

$$f(q_x) = \frac{C}{2} \left[ \frac{\sin[\pi Z \cot \delta (Q-q)_x]}{\pi Z \cot \delta (Q-q)_x} \right] \left( \frac{\sin \pi d (Q-q)_x}{\cos \pi d (Q-q)_x} \right). \quad (12)$$

The intensity distribution about superlattice reflections is then given by (11).

Computer plots for the intensity distributions about the direct spot and superlattice spots are shown in Fig. 7. Figures 7a and 7b are the intensity distributions about the direct spot and superlattice spots, respectively, for a crystal of 625\AA\ thickness. Figures 7c and 7d are the intensity distributions for a crystal of 1125\AA\ thickness. The thickness of the crystal affects the magnitude of the

$$\frac{\sin[\pi Z \cot \delta (Q-q)_x]}{\pi Z \cot \delta (Q-q)_x} \left( \frac{\sin \pi d (Q-q)_x}{\cos \pi d (Q-q)_x} \right),$$

factors in the intensity distribution functions and therefore affects
the peak heights of the satellites.

The detail around the center peak A of Fig. 7a is shown in Fig. 8 and consists of small maxima. The intensity of the small maxima decrease with increasing distance from the center peak. In the present case where the number of stacking faults contributing to the diffraction pattern N is taken equal to 500 (i.e. a selected area of λυ) the spacing of the small maxima is \((Nd)^{-1} = 10^4 \text{ cm}^{-1}\). Similar small maxima are predicted in the intensity distribution for superlattice reflections. These small maxima will not be observed in normal electron diffraction patterns, but with low angle electron diffraction techniques it may be possible to resolve these peaks.

As predicted in Section 2, the calculated intensity distributions for the direct spot have three strong maxima denoted by A (central maximum), B and C (side maxima). For the superlattice reflection, the peaks A, B and C are split and the splitting equals \(l/d\). Weaker subsidiary maxima at distances of \(n/d\) (n integral) from these main peaks also occur for direct and superlattice spots.

The side maxima B and C and their associated fainter subsidiary maxima are normally not observed in electron diffraction patterns from CuAu II since in almost all cases more than two strong beams are excited in the crystal. When the effects of more than two strong beams are taken into account, more side maxima will occur and the intensity of the central maximum A and its subsidiary maxima will be larger, with respect to any one of the increased number of side maxima. This may be shown qualitatively by means of the dynamical construction on the dispersion surfaces (Fig. 9), for the case of three strong beams at a
single stacking fault. Wave amplitudes corresponding to the three wave points $D_{(1)}$, $D_{(2)}$, and $D_{(3)}$ contribute to the central maximum A. There are six side maxima corresponding to wave points $D_{(1,2)}$, $D_{(1,3)}$, $D_{(2,1)}$, $D_{(2,3)}$, $D_{(3,1)}$, and $D_{(3,2)}$. The intensity at the center peak due to Fraunhofer effects at stacking faults will, therefore, be of the order of nine times greater than the intensity of one of the six side peaks. For N stacking faults the six side peaks and their subsidiary maxima will be similarly weakened with respect to the center peak system. In general, in CuAu II electron diffraction patterns, many more than three strong beams are excited so the effects of the side peaks will be small. The form of the intensity distributions about the direct and superlattice spots in Figs. 7a and 7b then agree with the intensity distributions in the diffraction pattern in Fig. 5 which was taken from a crystal of the order of 600Å thick.
VI. THE NORMAL REFLECTIONS

For the two beam approximation where the diffracted beam is a normal reflection, \{(200) or \{(220) type reflections in CuAu I\} the phase factor \( \alpha \) equals zero. The amplitudes of Eqs. \((5b)\), \((5c)\) and \((5d)\) are equal to zero (see Appendix to reference 2) and the intensity distribution is the Bragg peak of the perfect crystal. In general, more than two strong beams are excited. Figure 9 is a section of the dispersion surfaces for three strong beams, the direct beam, a superlattice diffracted beam denoted \( g \) and a normal diffracted beam denoted \( s \). The calculation of the wave function of the electron in a stacking faulted crystal for three strong beams is similar to that of Whelan and Hirsch\(^1\) and also Fitzgerald and Mannami\(^2\) for two strong beams.

The amplitude ratio for the wave functions in the shaded region of Fig. 1 is

\[ C(i,j) \exp^{i\alpha_h} = \frac{\phi_h(i,j)}{\phi_o(i,j)} \]  

(13)

where \( h \) may take the values 0, \( g \), \( s \) and \( i \) and \( j \) take the values 1, 2 and 3. When \( i = j \), \((i,j)\) becomes \((i)\). The amplitude ratios \( C(i,j) \) correspond to the wave points \( D(i,j) \) (Fig. 9). \( \alpha_h \) is the phase factor equal to \( 2\pi h \cdot R \) where \( R \) is the fault vector of the stacking fault.

At the exit surface below the stacking fault the wave function is

\[ \phi(R_e) = \sum_{i=1,2,3} \sum_{j=1,2,3} \sum_{h=0, g, s} \phi_h(i,j)(R_e) \exp(2\pi i h \cdot R_e) \]  

(14)
In this case the amplitudes $\psi_s^{(i,j)}(R_e)$ which contribute to the intensity distribution about the normal reflections are non zero for $c_s = 0$.

For example,

$$\psi_s^{(2,1)}(R_e) = \frac{c_s^{(2,1)} |c_o^{(1)}| |c_1^{(2)}|}{|c_s| |c_1|} \times e^{i\alpha_s} \Psi_{\tilde{r}} \exp\{2\pi i (K-K_o^{(1)}) \cdot r_s + (K_o^{(1)} - K_o^{(2,1)}) \cdot r\}$$

(15)

where $K_o^{(i,j)}$ is the wave vector connecting the wave point $D^{(i,j)}$ with the origin 0. $r_s$ and $r$ are position vectors on the entrance surface and at the stacking fault respectively,

$$|c| = \begin{vmatrix} 1 & 1 & 1 \\ c_s^{(1)} & c_s^{(2)} & c_s^{(3)} \\ c_s^{(1)} & c_s^{(2)} & c_s^{(3)} \end{vmatrix},$$

$$|c_o^{(1)}| = \begin{vmatrix} c_s^{(2)} & c_s^{(3)} \\ c_s^{(2)} & c_s^{(3)} \end{vmatrix},$$

$$|c_o^{(2)}| = \begin{vmatrix} c_s^{(2)} & c_s^{(3)} \\ c_s^{(2)} & c_s^{(3)} \end{vmatrix}.$$
It can be seen $\phi_s^{(2,1)}(\mathbf{R}_e)$ is non-zero for $\alpha_s = 0$. Therefore, if more than two strong beams are excited, satellites will be observed at normal reflections and the intensity distributions will be similar to that for the direct spot since $\alpha_s = 0$. This treatment also explains the slit-like intensity distribution about the (0002) reflection in the zinc sulphide crystals (containing a single stacking fault) examined by Fitzgerald and Mannani. For this reflection $\alpha$ is zero and the intensity distribution cannot be explained by the two beam treatment proposed in that paper.
VII. DISCUSSION

The validity of the column approximation used in this paper is the same as in the calculation of image contrast at crystal defects. The column approximation is used to find the wave function \( \psi \) at the exit surface of the crystal. For the image contrast of the anti-phase boundaries \( |\psi|^2 \) is calculated and for the intensity distribution in the electron diffraction pattern \( |(\text{the Fourier transform of } \psi)|^2 \) is calculated. The treatment presented in this paper, therefore, gives an explanation consistent with observation for both the image contrast and the resultant diffraction pattern from a periodic arrangement of anti-phase boundaries.

The calculations presented in this paper indicate that a periodic arrangement of stacking faults in a thin crystal will produce unusual intensity distributions about electron diffraction spots. In the case of electron diffraction effects in CuAu II alloy this contribution must be taken into account in addition to contributions from double diffraction \(^7\) and periodic modulation of the structure factor.\(^6,8\)

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REFERENCES

Fig. 1. Model of a crystal containing a stacking fault and showing the coordinate system.
Fig. 2. A section of the dispersion surfaces showing the relations between the wave points and vectors for a crystal containing a stacking fault.
Fig. 3. Model of a crystal containing a periodic arrangement of stacking faults.
Fig. 4. The unit cell of the CuAu II structure.
Fig. 5. Electron diffraction pattern from a thin CuAu II crystal film containing components from each of the CuAu II orientations. The film is in the (001) orientation.
Fig. 6. Diagram of the observed diffraction pattern from CuAu II alloy for the electron beam along [001].
Fig. 7(a). Computer plots of the intensity distributions about the direct spot and superlattice spots \( q_X = (K_t)_X \) and \( q_X = (K_t + g)_X \).

Direct spot: \( Z = 6.25 \times 10^{-6} \) cm, \( \alpha = \pi \), \( x = 0 \),

\[ x(1) = -x(2) = 1, \tan \theta_B = 10^{-2}, \]
\[ \cot \delta = 10^{-2}, \text{ extinction distance} \]
\[ (\Delta k_o)^{-1} = 5 \times 10^{-6} \text{ cm. } d = 2 \times 10^{-7} \text{ cm.} \]
Fig. 7(b). Computer plots of the intensity distributions about the direct spot and superlattice spots \( q_x = (K_t)_X \) and \( q_x = (K_t + g)_X \).

Superlattice spot: the parameters have the same values as for (a).
Fig. 7(c). Computer plots of the intensity distributions about the direct spot and superlattice spots \( q_X = (K_t)_X \) and \( q_X = (K_t + g)_X \).

Direct spot: \( Z = 1.125 \times 10^{-5} \) cm, the other parameters having the same values as in (a).
Fig. 7(d). Computer plots of the intensity distributions about the direct spot and superlattice spots \( q_X = (K_t)_X \) and \( q_X = (K_t + g)_X \).

Superlattice spot: the parameters have the same values as in (c).
Fig. 8. The region from \( q_x = -5 \times 10^4 \text{ cm}^{-1} \) to \( q_x = +5 \times 10^4 \text{ cm}^{-1} \) about the center peak A in Fig. 7(a) shown in greater detail.
Fig. 9. The dynamical construction for a stacking fault on the dispersion surface for three strong beams. $n_c$ is the normal to the crystal surface and $n_s$ is the normal to the stacking fault plane. $S_0$ is a circle of radius $X$ about 0 as center. $S_G$ and $S_S$ are circles of radius $X$ about $G$ and $S$ as centers. $G^*$ and $S$ are systematic reflections where $s = 2$ and $X$ is the wave vector of a kinematically reflected wave.
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