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Multiple diffraction origin of low energy electron diffraction intensities. II*. By R. M. STERN, A. GERVAIS and M. MENES, *Department of Physics, Polytechnic Institute of Brooklyn, Brooklyn, N. Y. 21201, U. S. A.*

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Strong minima in the rotation diagram about the 550 Bragg reflection from the (110) surface of tungsten are interpreted as being due to the excitation of forward diffracted Laue reflections having low index and large wave amplitude. The orientations of these minima correspond to the geometry for the excitation of the three beam case.

In a recent article (Gervais, Stern & Menes, 1968) the structure in the rotation diagrams from a tungsten (110) surface was interpreted in terms of multiple diffraction. At that time we were mostly concerned about what appeared to be strong, sharp maxima, attributing their origin to the presence of simultaneous reflections. A detailed systematic investigation of the nature and origin of the structure observed in rotation diagrams indicates that this interpretation was misleading; the multiple diffraction causes sharp minima in the intensity. This can be seen from the following qualitative argument. If a Bragg maximum is excited in the specularly reflected beam, then that reflection remains excited during a rotation about the surface normal. If no other reflections are considered to be excited, then during the rotation the incident beam remains totally reflected. When dynamical interactions are included the excitation of other reflections will cause a decrease in the specularly reflected intensity on the basis of conservation of current.

It is found that the origin of the minima in the rotation diagrams is the excitation of strong forward scattered Laue reflections, having for the most part an index $H(hkl)$ such that $h^2 + k^2 + l^2 \leq 12$. This conclusion is justified on the basis of the diffraction geometry determined by the incident beam orientation, and an analysis of the measured total secondary emission current from the crystal during both rotation diagrams and rocking curves.

In each case, the excitation of a low-index Laue reflection is accompanied by a strong reduction in the amplitude of the secondary emission and in the specularly reflected Bragg intensity. The mechanism for the reduction in the secondary emission is the reduction in the net absorption of the wave field propagating in the crystal during the excitation of the Laue reflection; the forward scattered beam carrying the field deep into the crystal. Secondary electrons produced far from the surface have a reduced escape probability and hence do not contribute to the secondary current (Stern & Taub, 1968).

That the Bragg intensity is reduced because of the large amplitude of the Laue wave field can be shown quantitatively by solving the secular equation in the three beam approximation of Bethe (1928); in particular the ratio of the plane wave amplitudes can be determined for a given geometry. It has been shown that for certain diffraction geometry the wave field amplitude associated with a sheet of the dispersion surface can become zero (Niehrs, 1954). Furthermore, Stern, Perry & Boudreaux (1969) have shown in the three-beam approximation for the mixed Bragg-Laue case, that there exist diffraction conditions for which the crystal-line plane wave associated with the specular Bragg reflection of a rotation diagram becomes zero.

Fig. 1 shows the orientations and indices of the Laue reflections which are excited during the rotation about the (550) reflection and which result in a reduction of the reflection coefficient (three beam case). The Figure also shows the orientations for Bragg reflections which reduce the

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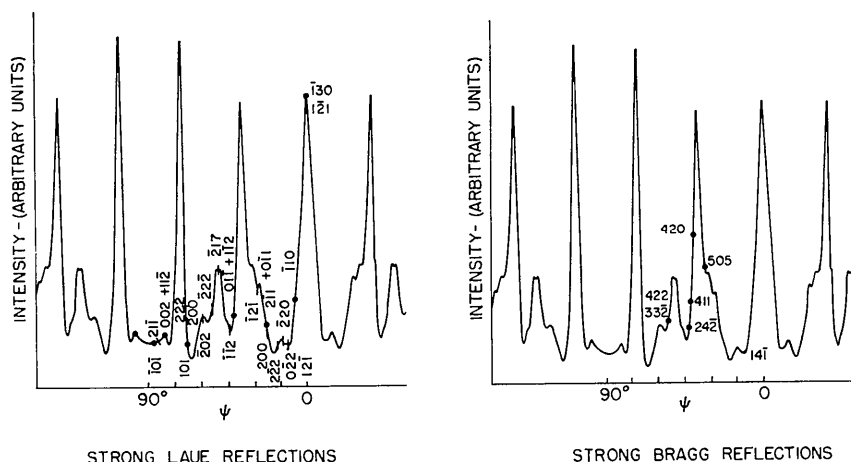


Fig. 1. Total integrated intensity of the specularly reflected beam *vs.* azimuthal angle (a rotation diagram) for the 550 reflection from the (110) surface of tungsten. $2\theta = 65^\circ$, $V = 547$ volts. Left hand diagram; the orientation of the plane of diffraction for the excitation of forward Laue reflections whose indices are shown. Right hand diagram; orientation for the excitation of Bragg reflections.

intensity of the specularly reflected beam (by conservation of current) but which do not affect the secondary current. Fig. 2 shows the total secondary current as well as the specularly reflected intensity for one quadrant of the rotation diagram about the (660) reflection. The minima in the secondary emission are associated with the geometry for the excitation of low index Laue reflections. The minimum in the specular reflection about the (002) orientation is due to a Bragg reflection and is not accompanied by a reduction in the secondary emission. In both Figures the strong minima occur for the excitation of Laue reflection belonging to the (110) zone.

The maxima in the reflected intensity, which occur when the incident plane is parallel to a low index plane of the crystal are partially an artifact due to the lack of Laue reflections which can be excited near to these orientations, and may also, in part, be due to a dynamical mechanism similar to that of the blocking observed for the scattering of heavy particles in these directions (Erginsoy, Datz, Leibfried & Lutz, 1967). The orientations of these low index planes also correspond to the centers of the Kikuchi bands associated with the same planes (Baudoing, Stern & Taub, 1968). The loci of the incident beam directions for the excitation of a Laue reflection (The Brillouin zone boundaries) are just the directions of the Kikuchi lines diffracted from the planes of the same index (optical reversibility or reciprocity theorem). A detailed analysis of rotation diagrams will appear elsewhere (Stern, 1968; Stern, Taub & Gervais, 1969; Stern, Gervais & Taub, 1969).

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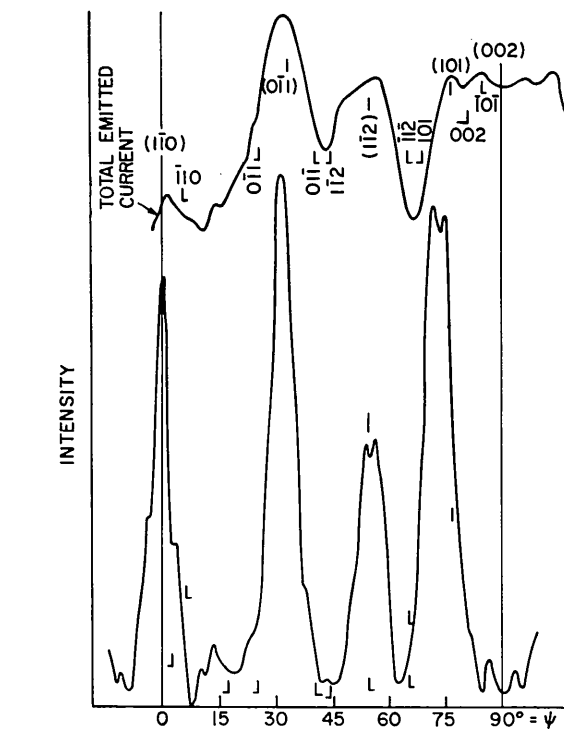


Fig. 2. Lower curve: Rotation diagram about the 660 reflection, $2\theta = 65^\circ$, $V = 825$ volts. Upper curve; total emitted secondary electron current as a function of azimuthal angle. The orientation of the dense planes of the (110) zone are indicated by short vertical lines. The orientation of the plane of incidence for the excitation of Laue reflections are shown by | and j, which bracket each of the low index planes. These orientations correspond to the position of the pair of Kikuchi lines from these planes.

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Diffraction symbols. Erratum. By J. D. H. DONNAY, *Crystallographic Laboratory, The Johns Hopkins University, Baltimore, Maryland 21218, U.S.A.* and OLGA KENNARD, *University Chemical Laboratory, Cambridge, England*

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In the paper published under the above title (Donnay & Kennard, 1964), please restore omitted words as follows:

Page 1340, column 1, line 3 up: *after the word aspect, insert $P3_{1,2}^{**}$ into.*

Note also that the space-group symbols used in this paper are those of the 1935 edition of the International Tables. Any screw axis that results from intersecting symmetry planes need not be explicitly symbolized, although this was done in the 1952 edition. Examples: $P4mc = P4_2mc$, $14md =$

14_1md , $Pbc2 = Pbc2_1$. The subscripts can easily be added by those who prefer the more explicit symbolism. We feel an explanation is in order, in view of the correspondence we received on this particular point.

Reference

- DONNAY, J. D. H. & KENNARD, O. (1964). *Acta Cryst.* **17**, 1337.