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**MULTIPLE-SCATTERING
DESCRIPTION OF INTENSITY
PROFILES OBSERVED IN
LOW-ENERGY-ELECTRON
DIFFRACTION FROM SOLIDS**

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This work was supported in whole by the Joint Services Electronics Program (U.S. Army, U.S. Navy, and U.S. Air Force) under Contract DAAB 07-67-C-0199

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MULTIPLE-SCATTERING DESCRIPTION OF INTENSITY PROFILES
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ABSTRACT

The dependence on beam energy and lattice geometry of the intensity of electrons diffracted from surfaces is evaluated using the inelastic-collision model. At energies below that of the second primary Bragg peak, qualitative features of the intensity profiles are related to the lattice geometry. Their quantitative features depend sensitively on the scattering from the surface layer. The first detailed interpretation of such profiles is proposed for the (100) face of tungsten.

*This work was supported in part by the Joint Services Electronics Program (Army, Navy, and Air Force) under Contract DAAB-07-67-C-1099.

In recent work we have presented a heuristic derivation¹, a perturbation-theory analysis², and a matrix-inversion analysis³ of the inelastic-collision model for the evaluation of the intensity versus energy profiles of low-energy electron beams diffracted from crystal surfaces. In this letter we summarize the major results of our analysis and note their consequences for the interpretation of experimental data.

Interest in this topic is due primarily to the fact that despite both numerous experimental measurements of intensity profiles since 1927⁴, and extensive theoretical studies of the effects of multiple-scattering^{2,5-14}, our results constitute the first systematic discussion of the dependence of the predictions of such models on the values of the model parameters and the first interpretation of experimental intensity profiles for low-energy electrons. Earlier attempted interpretations¹⁵⁻¹⁷ were based on a Darwin kinematical model in which the predicted scattering intensity is not simply related to a solution of the Schrödinger equation describing the electronic motion. Our analysis also reveals the critical importance for the interpretation of LEED profiles both of strong inelastic-collision damping and of the electronic inequivalence of the "surface" and "bulk" layers of even a chemically clean surface. Both of these effects previously have been regarded as "unimportant" in the current theoretical literature^{7-14,18} on multiple-scattering descriptions of LEED intensities.

The essential concept underlying the inelastic-collision model¹ is that the damping of the elastic wave field of an incident electron, due to its excitation of plasmons and incoherent electron-hole pairs, is the dominant feature of its motion in a solid which restricts its (elastic) penetration

into the solid to a depth of about 5-10 Å. In this limit,^{1,19} the energy widths and maximum intensities of the diffraction peaks are determined primarily by the damping length rather than by the lattice potential of the solid. The analytical formulation of the inelastic-collision model is achieved by using a propagator formalism¹³ to describe the multiple scattering by the lattice. The new feature of the model is the use of electron propagators associated with a (uniform) interacting electron fluid²⁰, rather than those associated with noninteracting electrons¹³. The final result¹⁻³ is an expression for the intensity of a given LEED beam as a function of (1) its energy, E , (2) its momentum parallel to the surface of the crystal, k_{\parallel} ; and (3) the ion-core partial-wave scattering amplitudes and (energy-dependent) electronic proper self energy characteristic of the target.

In this letter we consider only the (00) diffracted beam using a simplified, semiphenomenological version² of the inelastic-collision model in which the ion-core scattering is described by an s-wave scattering amplitude

$$t(E) = \{ \exp [2i\delta(E)] - 1 \} / 2ik(E) \quad [1]$$

and the electronic proper self energy is taken to be

$$\Sigma(K, E) \equiv V_o(E) - i\Gamma(E) \quad [2]$$

in which V_o is the electron inner potential and $\Gamma(E)$ is related to a prescribed damping length, λ_{ee} , by

$$\Gamma(E) \equiv \frac{\hbar^2}{2m\lambda_{ee}} \left[\frac{2m}{\hbar^2} (E + V_o) \right]^{\frac{1}{2}}. \quad [3]$$

The propagation wave vector in the solid is determined by energy and $\tilde{k}_{||}$ conservation via

$$E - \frac{\hbar^2}{2m} (k_{\perp}^2 + k_{||}^2) - \Sigma(k_{\perp}, \tilde{k}_{||}, E) = 0. \quad [4]$$

Equation [4] leads to a complex propagation constant, $k_{\perp} = k_{\perp 1} + ik_{\perp 2}$, for motion normal to the surface of the crystal.

The intensity of the (00) diffracted beam is a function of the beam parameters, E and $\tilde{k}_{||}$, and of the material parameters δ_S, δ_B , and λ_{ee} . A subscript S is used to designate the phase shift associated with ion cores in the surface layer and a subscript B to designate the remaining "bulk" ion core phase shifts. It is given by^{1,13}

$$I_{00}(E) = \left| \frac{-m}{2\pi\hbar^2} \sum_v e^{2ik_{\perp}(E)d_v} T_v \delta_{\tilde{k}'_{||} \tilde{k}_{||}} \right|^2 \quad [5]$$

in which d_v denotes the distance from the surface of the layer labeled by v [$v = 0$ denotes the surface layer]. The self-consistent layer scattering amplitudes T_v satisfy a set of coupled algebraic equations^{1,13} of the form

$$T_v = \tau_v + \tau_v \sum_{v' \neq v} G_{vv'} T_{v'} \quad [6a]$$

$$T_v = t_v [1 - t_v G_v]^{-1} \quad [6b]$$

in which $G_{vv'}$ and G_v are appropriately defined propagators^{1,2,13}. Thus τ_v describes the scattering from an isolated " v^{th} " layer of ion-cores.

It exhibits resonance structure [for s-wave scattering] when $[1-t_v G_v]^{-1} \rightarrow 0$. These Resonances have been designated "multiple-scattering" resonances by McRae⁷. They correspond to a threshold effect in an elastic channel near the threshold for an inelastic process². The conventional " n^{th} -order primary Bragg peaks" result from taking all of the T_v to be identical constants. Additional resonant peaks and minima in $I_{oo}(E)$ occur because $T_v \neq \tau$ in the solutions of Eq. [6a]. We refer to them as "higher-order" Bragg peaks. The criteria for these higher-order peaks depends both on the Bravais net parallel to the surface and on the geometry of successive scattering planes². Hence, the energy at which they occur is a direct and rather sensitive consequence of the geometry of the ion-core arrangement in the top few layers of the solid².

The first task in an investigation of the consequences of our model is the determination of the dependence of the predicted intensity profile on the values of the model parameters. The theory of the uniform electron fluid^{1,20} predicts that $\lambda_{ee}(e)$ decreases from nearly infinity at the Fermi energy in the solid, to a value of about 4-6 Å at energies near ten times the Fermi degeneracy, ζ , and then slowly increases with increasing energy. This predicted behavior is consistent¹ with all known data on the inelastic-collision mean-free paths of electrons in the energy range $E \lesssim 200$ eV. The inner potential is known to satisfy²¹ $V_o(\mu) = -\phi - \zeta$ for electrons at the Fermi energy, μ , where ϕ is the field-emission work function and ζ is the Fermi degeneracy of the valence electrons. Except near a plasmon-emission threshold, $V_o(E)$ decreases in magnitude with increasing energy^{20,21}. The ion-core phase

shifts are not known, but in principle can be related to the parameters of models for the ion-core potentials. The extreme sensitivity of the predicted intensity profiles to the values of these phase shifts is illustrated in Fig. 1. From this figure and similar calculations we conclude that the electronic structure of the ion-core factors in the top layers of the solid usually dominates the predicted intensity profiles. Hence LEED intensity profiles do not reflect the band structure of the bulk solid, but rather measure the electronic properties of the surface layers. In metals, the electronic structure/bulk and surface layers differ even for chemically clean surfaces²¹. The great importance of the electronic inequivalence of the surface and bulk layers for the prediction of intensity profiles renders "first-principles" calculations of these profiles considerably less reliable than those of bulk electronic band structures, because of the difficulty in describing variations in the electronic density (and hence ion-core-form factors) in the top layers of the solid²¹.

A detailed discussion of the influence of the lattice geometry on the intensity profiles is given by Duke, Anderson, and Tucker². The important feature of this discussion is its simplicity which renders the results directly useful by experimentalists. As the simplicity of this analysis relies heavily on the use of double-diffraction perturbation theory², we have compared the intensities thus calculated with those obtained from the numerical solution of Eqs. [6]. The results for three faces of aluminum are shown in Fig. 2. The usual consequence of the numerical calculation, evident in the figure, is the smoothing out of some of the fine structure predicted by the double-diffraction approximation. However, the qualitative features of the predicted intensity profiles remain unaltered for s-wave scattering from equivalent layers of ion-cores. The case of an inequivalent surface layer is more complicated and is currently under study³.

Concluding with the question of the interpretation of experimental data, we first note that the relation between lattice geometry and the features of the intensity profile is likely to be simply only at energies below that of the $n=2$ primary Bragg peak, unless the electron ion-core scattering is sufficiently weak that only primary Bragg peaks occur at higher energies. The most extensive low-energy data/^{on metals} has been taken on the (110), (100), and (211) faces of Tungsten^{15, 22-25}. A discussion of all three faces is given by Duke, Anderson and Tucker². In Fig. 3 we show a comparison between the model calculations and experimental data at two angles of incidence on W(100). The qualitative similarity between the theoretical and experimental profiles is evident from the figure. The interpretation of the maxima in the calculated profiles is noted in the figure. Although small changes in the parameters δ_S , δ_B and λ_{ee} do not alter drastically the calculated intensities, the suitability of the theoretical description was decreased substantially by the use of other regions of the three-dimensional parameter space which we searched. The deviations evident in Fig. 3 between the experimental data and the model predictions are comparable to the deviations between experimental measurements taken on different, "equivalent" crystals²²⁻²⁵. Therefore we conclude that the interpretations noted in Fig. 3 are reasonably unique consequences of the double-diffraction analysis of the model, although the associated inner-potential shifts, $V_o \approx 5\text{eV}$, are smaller than we anticipated.

The numerical solutions to Eqs.[6] for a normally-incident beam give results³ similar to those shown in Fig. 3 with the $n=1$ Bragg peak apparently occurring as a high-energy shoulder on the multiple-scattering structure.

Another large maximum occurs near 28 eV. The only sensible alternative to the interpretation given in Fig. 3 seems to be that obtained by identifying the experimental observations with this higher-energy resonance and using an inner potential $V_o \approx 20$ eV. Hence the interpretation in Fig. 3 appears to be the more reasonable one of the two alternatives.

The authors gratefully acknowledge helpful correspondence with Dr. P. J. Hobson and Professor F. M. Propst. We are indebted to Professor Propst for permission to use his unpublished data.

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FIGURE CAPTIONS

- Fig. 1 - Intensities of the (00) beam normally incident on the (100) face of a simple cubic lattice calculated in second-order perturbation theory. Scattering from the top layer of ion cores is described by the phase shift δ_S and that from the "bulk" ion cores by δ_B . The intensities are calculated using Eqs. [15], [30], [44], and [45] given by Duke, Anderson and Tucker² using the parameters shown in the figure.
- Fig. 2 - Comparison of the matrix-inversion and double-diffraction calculations of a (00) beam of electrons normally incident on the various faces of an (fcc) aluminum lattice. The parameters used in the calculations are indicated in the figure. In all cases, the results of the matrix inversion calculations do not change significantly if the dimensionality of the matrix is increased further.
- Fig. 3 - Comparison of the intensity profiles calculated using the double-diffraction approximation (top panels) with the experimental relative intensity profiles (lower panels) for a (00) beam incident on the (100) face of tungsten. The identification of the various peaks in the calculated profiles is indicated. The values of the phase shifts were adjusted to describe the data. The calculations were performed using Eqs. [15], [30], [44] and [45] in Duke, Anderson, and Tucker². The normal-incidence experimental data are taken from Khan, Hobson, and Armstrong²² and the 53° incidence data from Propst²⁵.

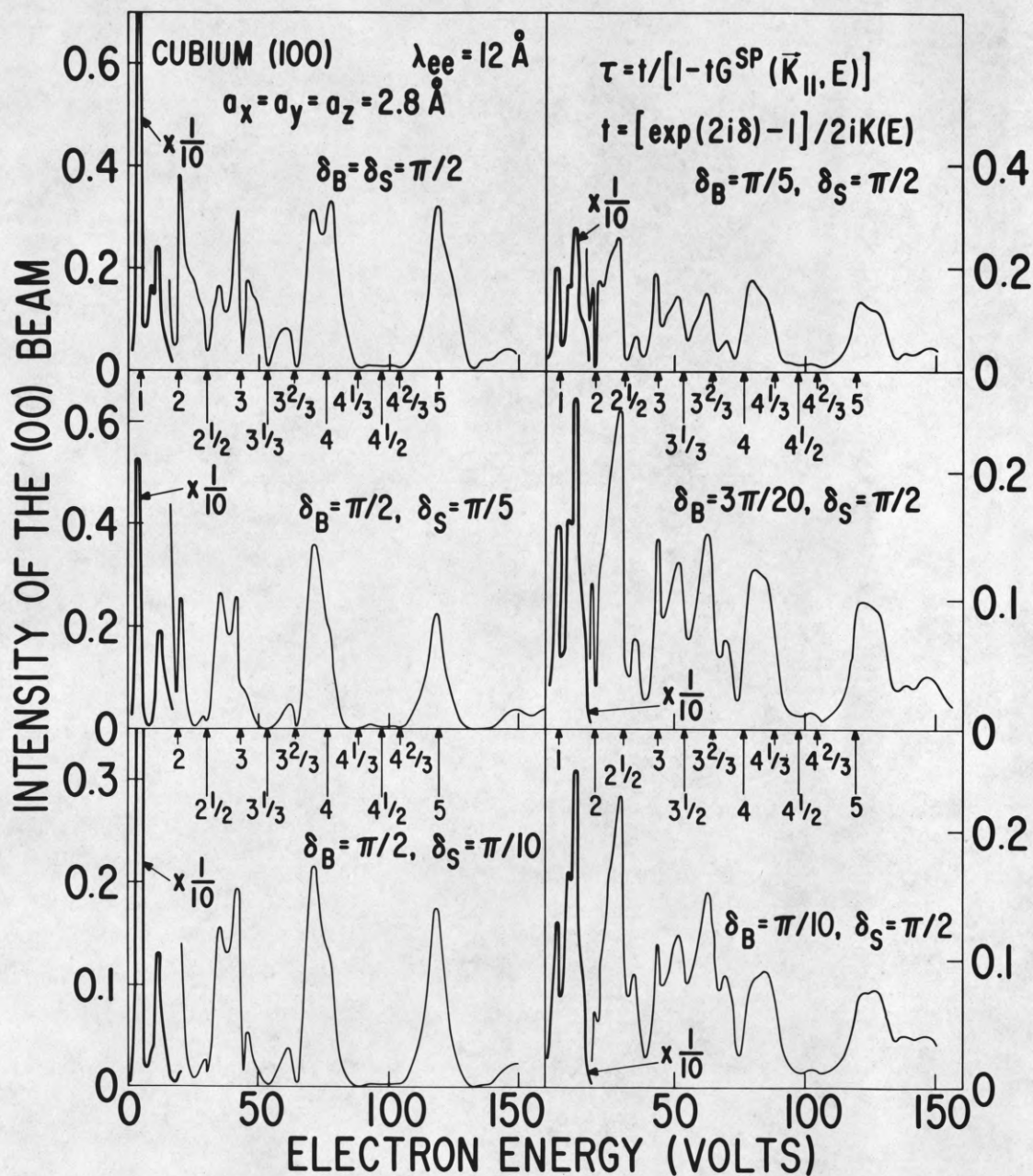


Figure 1

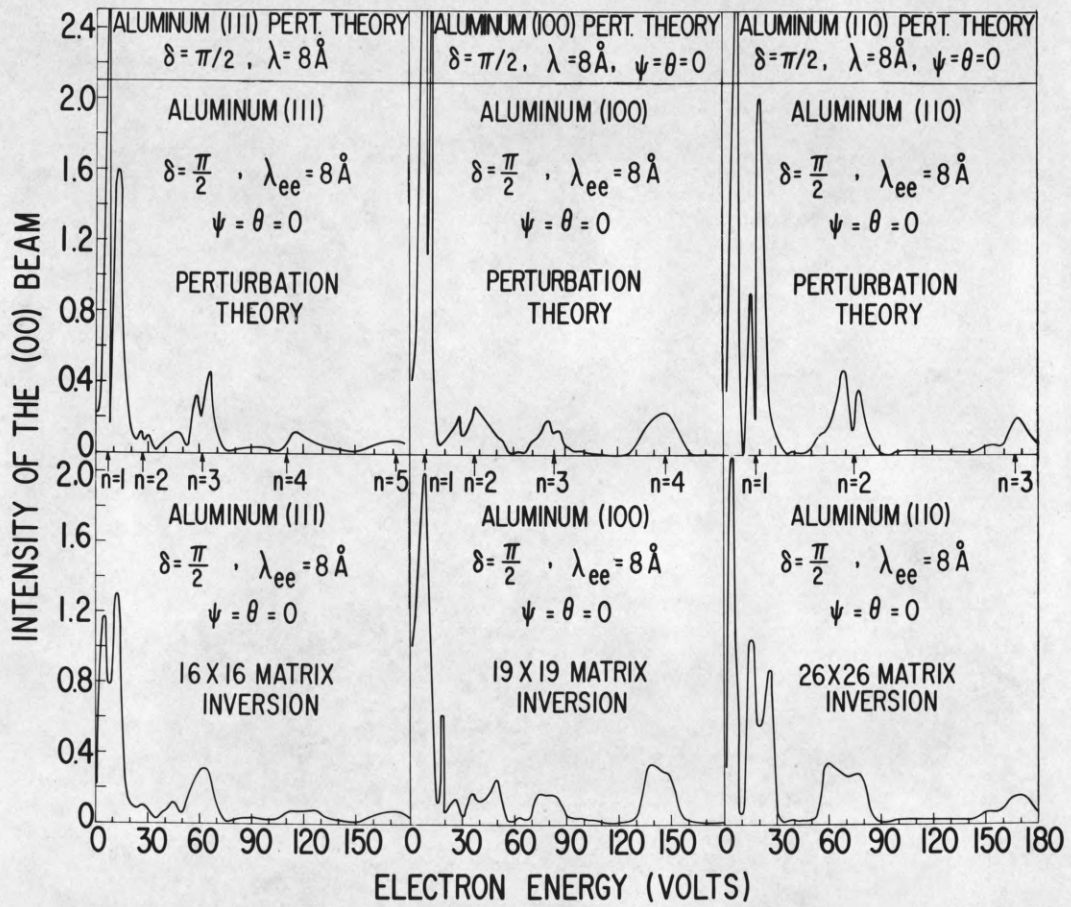


Figure 2

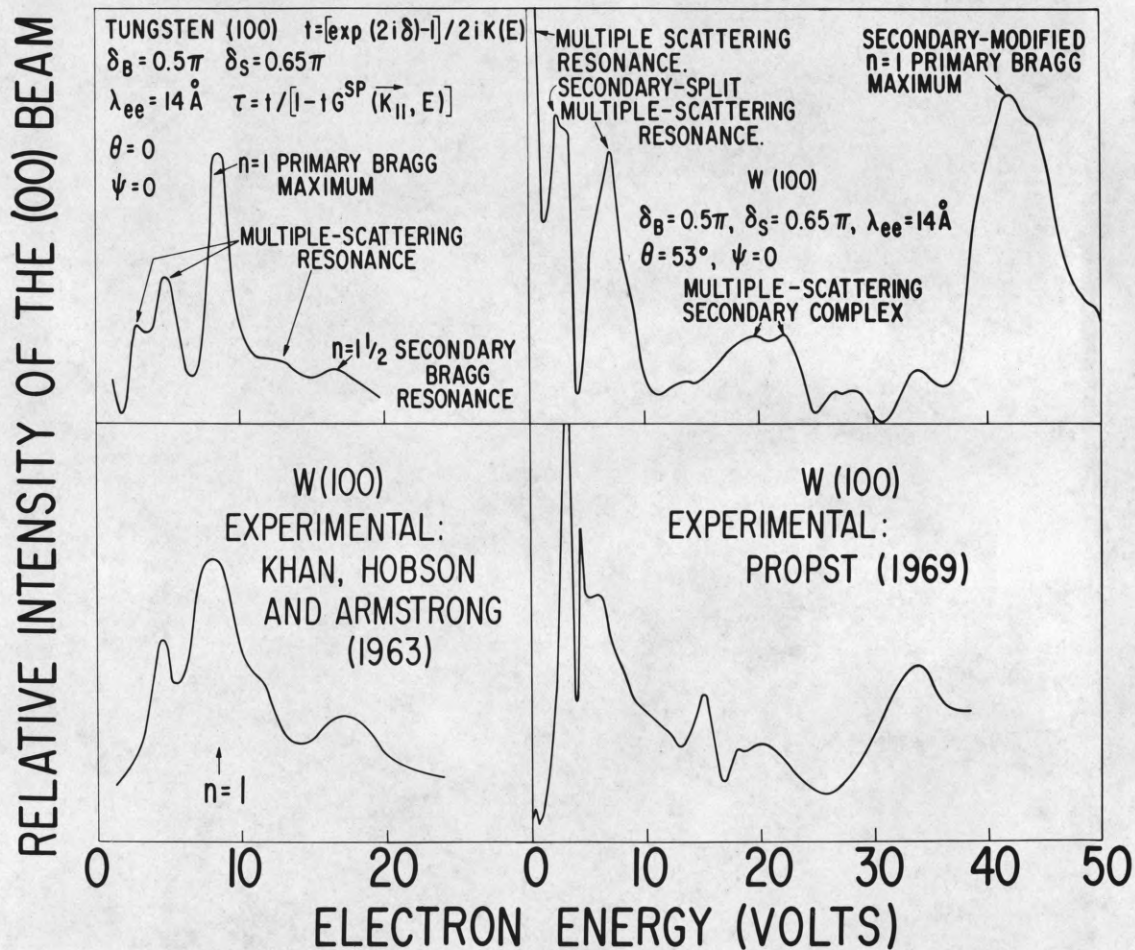


Figure 3

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DOCUMENT CONTROL DATA - R & D

(Security classification of title, body or abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author)

University of Illinois
Coordinated Science Laboratory
Urbana, Illinois 61801

2a. REPORT SECURITY CLASSIFICATION

Unclassified

2b. GROUP

3. REPORT TITLE

MULTIPLE-SCATTERING DESCRIPTION OF INTENSITY PROFILES OBSERVED IN LOW-ENERGY-ELECTRON
DIFFRACTION FROM SOLIDS

4. DESCRIPTIVE NOTES (Type of report and inclusive dates)

5. AUTHOR(S) (First name, middle initial, last name)

DUKE, C. B. , TUCKER, C.W., Jr

6. REPORT DATE

September, 1969

7a. TOTAL NO. OF PAGES

12

7b. NO. OF REFS

25

8a. CONTRACT OR GRANT NO.

DAAB 07-67-C-0199

b. PROJECT NO.

9a. ORIGINATOR'S REPORT NUMBER(S)

R-431

9b. OTHER REPORT NO(S) (Any other numbers that may be assigned
this report)

10. DISTRIBUTION STATEMENT

This document has been approved for public release and sale; its distribution is
unlimited.

11. SUPPLEMENTARY NOTES

12. SPONSORING MILITARY ACTIVITY

Joint Services Electronics Program
thru U.S. Army Electronics Command
Fort Monmouth, New Jersey 07703

13. ABSTRACT

The dependence on beam energy and lattice geometry of the intensity of electrons diffracted from surfaces is evaluated using the inelastic-collision model. At energies below that of the second primary Bragg peak, qualitative features of the intensity profiles are related to the lattice geometry. Their quantitative features depend sensitively on the scattering from the surface layer. The first detailed interpretation of such profiles is proposed for the (100) face of tungsten.

KEY WORDS

LINK A

LINK B

LINK C

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Surface Physics

Electron Diffraction

Electron Scattering