Dynamic diffractive focusing of intermediate-energy electrons in a crystal and possible use of this effect for analyzing surface layers

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A focusing of a beam of intermediate-energy electrons in a crystal has been observed. A method based on this effect is proposed for analyzing surface layers. The idea is to record spectra of secondary processes by varying the voltage accelerating the beam.

The mean free path of intermediate-energy electrons (with a kinetic energy $E \sim 10$ keV) is comparable in order of magnitude to the corresponding extinction lengths,[1] so the electron wave field near the surface of a crystal is determined to a large extent by a coherent interference by electron Bloch waves. Experimental evidence for this assertion comes from the anisotropy of the Auger emission which is seen as the angle of incidence of the beam is varied (Ref. 2, for example).

At these energies, the motion of the particles can be described completely satisfactorily in a crystal potential which is averaged over the direction of incidence of the beam. In other words, the basic physical characteristics of Bloch states j, specifically, their populations $\epsilon^{(j)}$ and their transverse energies $E_\perp^{(j)} = E - (\hbar k_z^{(j)})^2/2m$, can be calculated sufficiently accurately in the approximation of the zeroth Laue zone of the theory of multiwave dynamic diffraction. The latter properties are determined from the projections of the wave vectors $k^{(j)}$ onto the normal (z) to the surface of the crystal (Fig. 1).

Although the diffraction of electrons is generally of a substantially multiwave nature, because the electron wavelength is small in comparison with the interatomic distance,[3] when a beam is incident along a crystallographic axis, the number of waves is effectively reduced. The reason is that the selection rules[4] state that the Bloch states of only a single irreducible representation of the symmetry group of the problem (s states in a hydrogen-like classification[5]) can be populated. The degree of divergence of the beam or its deviation from the crystallographic axis was studied in Ref. 6. On the other hand, the potential wells are very shallow at these energies, and they generally hold no more than one or two bound-motion levels. Since only bound or valence states ($E_\perp^{(j)} \lesssim -V_0$, where V_0 is the average internal potential in the crystal) can be highly occupied, because of the attractive effect of the atomic chains on the electrons,[7–9] it is easy to see that the wave field in the crystal may be determined highly accurately by only two or three Bloch waves under these conditions (Fig. 1, for example). The result is a fairly simple modulation of the electron beam by the crystal lattice inside the crystal. For example, the modulation would be sinusoidal if there were two highly populated states.

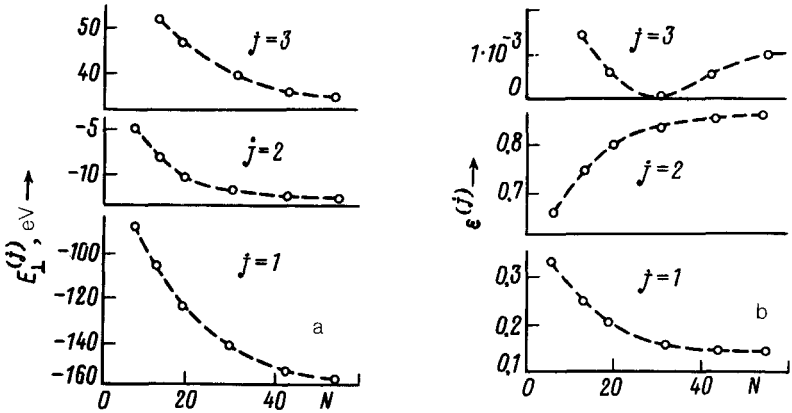

FIG. 1. (a) The transverse energies $E_\perp^{(j)}$ and (b) the populations $\epsilon^{(j)}$ of the first three electron Bloch states, $j = 1, 2, 3$, in ⟨111⟩ Mo at $E = 10$ keV versus the number (N) of diffracted beams which are incorporated correctly in the approximation of the zeroth Laue zone of the theory of multiwave dynamic diffraction.

The highly populated bound and valence states are evidently also highly localized at the atomic chains (Fig. 2), so at the depths at which they come into phase the density of the electron beam on a chain may reach a level many times the density of the incident particles. This circumstance, combined with the pronounced loss of coherence due to inelastic processes, allows us to speak in terms of a dynamic diffractive focusing in this case. If there are two highly populated states (Fig. 3), for example, this focusing would occur at a thickness $z_f = 1/2(k^{(1)} - k^{(2)}) \approx \sqrt{(E + V_0)h^2/2m}/(E_\perp^{(2)} - E_\perp^{(1)})$.

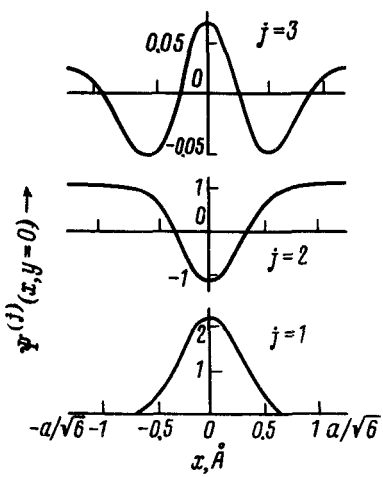

FIG. 2. Cross sections of the distributions $\Psi^{(j)}(x,y = 0)$ of the first three electron Bloch states, $j = 1, 2, 3$, in the unit cell of ⟨111⟩ Mo (the lattice constant is $a = 3.14$ Å) for $E = 10$ keV, as calculated from 55 diffracted beams.

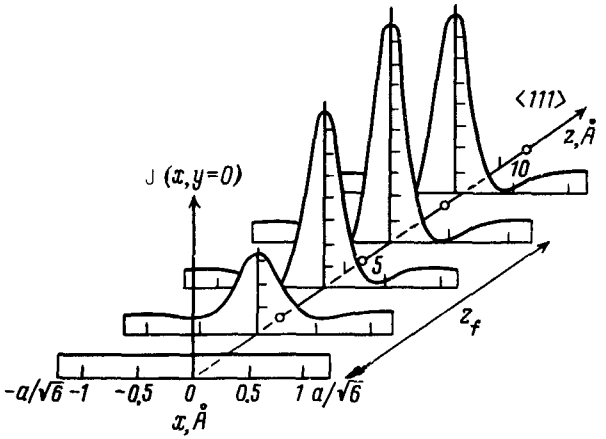

FIG. 3. Arrangement for varying the density of the electron beam in the unit cell of ⟨111⟩ Mo along depth in the crystal, z, at $E = 10$ keV. The points are the positions of atomic planes along the ⟨111⟩ axis.

At the energies under consideration here, the values of z_f are comparable in order of magnitude to a few interatomic distances, so a change in the accelerating voltage would change the focal length $z_f(E)$. This change would in turn lead to a variation in the flux density of the incident particles on the atomic planes of the crystal. The intensity of the secondary processes accompanying the passage of the electron beam through the crystal would thus become oscillatory. This oscillatory dependence would evidently become more obvious in thin samples, i.e., with increasing degree of coherence of the wave field in the crystal, and also if the accelerating voltage were not too high, so that the modulation period of the electron beam did not span an overly large number of atomic planes.

By varying the accelerating voltage under the conditions required for this focusing effect, one can actually scan over the thickness of a crystal. It thus becomes possible to work from the characteristic spectra of the secondary processes to extract information on not only the nature of the defects in the surface layer but also the depths of these defects. It apparently might also be possible to utilize this effect to determine the thicknesses of thin single-crystal films, including multilayer structures. It might be used to determine the polarity of a crystal. Data on the spatial distribution of cathodoluminescence centers in an atomic lattice might provide useful information about the nature of these centers.

This new method is conceptually close to the method of standing x-ray waves,[10] with the distinction that the position of the region of elevated density of the incident beam in the crystal is varied in the present case not by varying the angle of incidence of the beam on the crystal but by varying the voltage which accelerates the beam. The significantly greater degree of localization of the beam on the atomic planes in this case is important.

[1]L. C. Feldman and J. W. Mayer, *Fundamentals of Surface and Thin Film Analysis*, Elsevier, New York, 1986.

[2]A. I. Kovalev and G. V. Shcherbedinskiĭ, *Modern Methods For Studying the Surfaces of Metals and Alloys*, Metallurgiya, Moscow, 1989.
[3]J. Cowley, *Physics of Diffraction* [Russian translation], Mir, Moscow, 1979.
[4]F. N. Chukhovskii and V. L. Vergasov, Acta Crystallogr. A **46**, 153 (1990).
[5]S. A. Vorob'ev, *Channeling of Electron Beams*, Energoatomizdat, Moscow, 1984.
[6]V. L. Vergasov and F. N. Chukhovskiĭ, Izv. Akad. Nauk SSSR Ser. Fiz. **48**, 1671 (1984).
[7]F. Fujimoto, in *Proc. Fifth Int. Congr. on HVEM*, Kyoto, 1977, p. 271.
[8]Yu. Kagan, E. A. Babakhanyan, and Yu. V. Konenets, Pis'ma Zh. Eksp. Teor. Fiz. **31**, 776 (1980) [JETP Lett. **31**, 733 (1980)].
[9]V. L. Vergasov and F. N. Chukhovskii, Phys. Lett. A **110**, 228 (1985).
[10]A. M. Afanas'ev, P. A. Aleksandrov, and R. M. Imamov, *x-Ray Diagnostics of Submicron Layers*, Nauka, Moscow, 1989.

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