X-ray surface waves

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It is shown that for small angles of incidence of x-ray radiation on a single crystal, diffraction in the surface layer leads to the formation of surface waves with the following structure: the intensity is maximum at the separation boundary and decays on both sides of it.

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This paper is concerned with an investigation of the properties of total external reflection (TER) from single crystals. It is shown that dynamic diffraction in the surface layer in a system of surfaces perpendicular to the input face of the crystal leads to the appearance of a diffracted surface wave which decays into the bulk of the crystal as well as into the vacuum and which has an anomalous coefficient of absorption along the surface. The conditions for the appearance of the surface wave are determined.

The condition for the appearance of surface waves at the boundary separating the vacuum and the medium has the form[1] $\epsilon(\omega,\mathbf{k}) < -1$. The negative dielectric constant stems from the damping of the wave into the bulk of the medium, while the condition $|\epsilon| > 1$ ensures that the wave vector in the vacuum is complex. In the x-ray range, the dielectric constant has the form $\epsilon_x = 1 - \delta$, where the quantity $\delta \sim 10^{-5}$, so that it would appear that there is no hope for the appearance of x-ray surface waves. However, it is shown in what follows that there is such a possibility. Since $\epsilon_x < 1$, damping of the wave into the bulk of the crystal can be achieved by exciting it under TER conditions. In order for the wave to be damped into the vacuum, it is necessary to satisfy the condition $|\epsilon_x| > 1$, which is attained under conditions of dynamic diffraction, since for the diffracted wave within the limits of the Bragg maximum, $\epsilon_x(\mathbf{k})$ can be less as well as greater than unity. For diffraction under TER conditions, it is therefore possible to excite in the direction of the diffracted wave a surface x-ray wave on the planes of the crystal perpendicular to the input face by choosing the excitation point.

Let us determine the conditions for the appearance of a surface x-ray wave. They follow from the continuity of the tangential components of the wave vectors at the separation boundary and the dispersion equation for two-wave diffraction in the medium. The mutual position of the wave vectors of the waves in the vacuum and in the medium are shown in Fig. 1. The indices $\vec{\kappa}$ indicate wave vectors of waves propagating in the vacuum, while $\mathbf{k}$ indicate waves propagating in the medium. Let the vector $\mathbf{H}_h$ be parallel to the surface of the crystal. Then, the projection of the wave vectors of the incident $\vec{\kappa}$ specularly reflected $\vec{\kappa}_0$, and the waves $\mathbf{k}_0,\mathbf{k}_h$ dynamically coupled in the crystal on the axis of the system of coordinates chosen by us can be written in the form

$$\vec{\kappa} = \{\kappa \sin\theta_0 \cos(\varphi - \eta), -\kappa \sin\theta_0 \sin(\varphi - \eta), \kappa \cos\theta_0\}$$

$$\vec{\kappa}_0 = \{\kappa \sin\theta_0 \cos(\varphi - \eta), -\kappa \sin\theta_0 \sin(\varphi - \eta), -\kappa \cos\theta_0\}, \qquad (1)$$

$$\vec{k}_0 = \{ \kappa \sin\theta_0 \cos(\varphi - \eta), -\kappa \sin\theta_0 \sin(\varphi - \eta), \quad \kappa\cos\theta_0 - \Delta \}$$

$$\vec{k}_h = \{\kappa \sin\theta_0 \cos(\varphi - \eta), \ H - \kappa \sin\theta_0 \sin(\varphi - \eta), \quad \kappa \cos\theta_0 - \Delta \}$$

where $\mathbf{H}_h = \{0, H, 0\}$, $\kappa = \omega/c$, η is the polar detuning angle from the exact Bragg angle, and $\vec{\Delta} = \{0, 0, {}^-\Delta\}$ is the refraction vector In the two-wave approximation, the solution of the standard dispersion equation leads to four values of Δ_i ($i = 1,2,3,4$). However, for a semi-infinite crystal, only the following two values are physically significant:

$$\Delta_i = \kappa \cos\theta_0 - \left[k^2 - \kappa^2 \sin^2\theta_0 - \frac{\kappa^2 a}{2} \pm \kappa^2 \sqrt{\frac{a^2}{4} + (4\pi C)^2 \chi_{\bar{h}} \chi_h} \right]^{1/2}, \quad (2)$$

where $k^2 = \kappa^2(1 + 4\pi\chi_0) = \kappa^2\epsilon$, C is the coefficient of polarization, χ_0, χ_h are the Fourier coefficients of the polarizability of the crystal, and

$$a = \frac{2H}{\kappa} \left[\frac{H}{2\kappa} - \sin\theta_0 \sin(\varphi - \eta) \right] \approx 2\eta \sin 2\varphi \sin^2\theta_0 . \quad (3)$$

Thus, under TER conditions in the crystal, waves can propagate with vectors k_{0i} and k_{hi} ($i = 1,2$), corresponding to the two dispersion surfaces.

$$k_{0i}^2 = \kappa^2 \left(\epsilon - \frac{a}{2} \pm \sqrt{\frac{a^2}{4} + (4\pi C)^2 \chi_{\bar{h}} \chi_h} \right) = \kappa^2 \epsilon_{0i} ,$$
$$k_{hi}^2 = \kappa^2 \left(\epsilon + \frac{a}{2} \pm \sqrt{\frac{a^2}{4} + (4\pi C)^2 \chi_{\bar{h}} \chi_h} \right) = \kappa^2 \epsilon_{hi}, \quad (4)$$
$$k_{0zi} = k_{hzi} = \kappa \sqrt{\epsilon_{0i} - \sin^2\theta_0} .$$

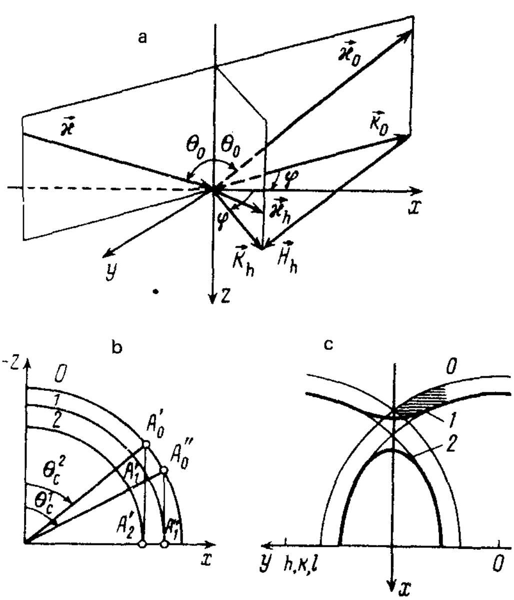

FIG. 1a. Geometry of diffraction of x rays at small glancing angles; the wave vectors correspond to the following waves: $\vec{\kappa}_0$ is the specularly reflected wave, $\mathbf{k}_0$ is the refracted wave, $\mathbf{k}_h = \mathbf{k}_0 + \mathbf{H}_h$ is the diffracted wave, and $\vec{\kappa}_h$ is the vacuum diffracted wave.

FIG. 1b. Section of the dispersion surface by the plane α = const; "0" is the trace of the kinematic sphere centered at the origin of the reciprocal lattice; "1" ("2") is the trace of the upper (lower) sheet of the dispersion surface for one of the polarizations; A_i are centers of excitation of the waves.

FIG. 1c. Section of the dispersion surface by the plane parallel to the input face of the crystal; the shaded region indicates the excitation points, for which the magnitude of the wave vector of the diffracted wave is greater than $\kappa = \omega/c$.

In contrast to a uniform medium, TER of x-rays from the crystal is characterized by two angles for each polarization of radiation ($\sin\theta_{ci} = \sqrt{\epsilon_{0i}}$), rather than by one critical angle θ_c. This circumstance was, apparently, first pointed out in Ref. 2. As is evident from Fig. 1b, the structures of the wave fields in the medium and in the vacuum differ strongly in the following three regions of values of θ_0: for $\theta_0 < \theta_{c2}$, all waves k_{0i} and k_{hi} propagate into the bulk of the crystal. For $\theta_{c2} \leqslant \theta_0 < \theta_{c1}$, only waves corresponding to one of the centers of excitation propagate into the crystal. Waves corresponding to the second center of excitation propagate parallel to the crystal surface, decaying into the crystal. For $\theta_0 \geqslant \theta_{c1}$, all four waves k_{0i}, k_{hi} propagate along the surface. Thus, for $\theta_0 \geqslant \theta_{c2}$, a new wave $-\vec{\kappa}_h$ is excited in the vacuum (Fig. 1a), whose direction of propagation is determined from the condition of continuity of the tangential component of the wave vector. Therefore, in the system of coordinates chosen by us, $\vec{\kappa}_h$ has the following components:

$$\vec{\kappa}_h = \{ \kappa \sin\theta_0 \cos(\varphi - \eta),\ H - \kappa \sin\theta_0 \sin(\varphi - \eta),\ -\kappa \cos\theta_h \}, \tag{5}$$

where

$$\cos\theta_h = \sqrt{\cos^2\theta_0 - a}\ . \tag{6}$$

The most important result of the last equation is the fact that for $a > \cos^2\theta_0$ and $\theta_0 \geqslant \theta_{c1}$, a surface wave, damped both into the crystal and into the vacuum, arises in the direction k_h. The geometrical location of the points of excitation, for which this situation arises, is the shaded area in Fig. 1c. It is easy to see that for values of χ_h close to χ_0, the region of excitation of surface waves lies within the range of the Bragg maximum. One of the results of this is a decrease in the coefficient of absorption (μ) of that part of the surface wave which propagates in the medium and under certain conditions of diffraction we will have for it $\mu \ll \mu_0$, where μ_0 is the normal photoelectric absorption coefficient.

The results obtained by us can be directly extended to the case of Mössbauer emission as well.

In conclusion, it may be assumed that future investigations of x-ray surface waves in different media and of the characteristics of their scattering by a separation boundary will lead to the development of a unique method for studying the real structure of the surface.

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