Nature of anomalous x-ray reflection from a surface

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The nonspecular peak in the angular spectrum of the x radiation reflected from a rough surface is shown to be caused by the formation of standing waves in the initial and final states of the scattered x rays at glancing angles close to the angle of total external reflection.

1. The anomalous reflection of x rays, i.e., the appearance near the angle of total external reflection of a nonspecular peak in the angular spectrum of the radiation scattered by a rough surface, was discovered experimentally 25 years ago.[1] Similar peaks have recently been seen in the angular spectra of x-ray fluorescence[2] and the thermal diffuse and Compton scattering of x rays.[3] The existing theory on anomalous reflection[4,5] is of a model nature and does not explain the basic physical reason for the appearance of a nonspecular peak in a wide range of experiments with x rays and γ rays.[1,4–6] The contradiction between the choice of an average value of the dielectric constant and the statistics of surface irregularities has led to some nonphysical features (in particular, a δ-function singularity has appeared in the direction of specular reflection) in the angular spectrum of the diffusely scattered radiation in some studies which have been reported.[7,8]

In this letter we offer an explanation for the appearance of a nonspecular peak in the angular spectrum of x rays reflected from a rough surface. The reason is a spatial redistribution of the fields of the incident and scattered radiation at glancing angles close to the critical value. The anomalous peak is made up of scattered waves which have field antinodes at the vacuum-medium interface.

2. We assume that the vacuum-medium interface is a random surface on which there is an abrupt change (over a distance on the order of atomic distances) in the dielectric constant.[9] The ideal surface coincides with the $z=0$ plane. The real vacuum-medium interface is described by an equation $z=\xi(x,y)$ where $\xi(x,y)$ is a random function with $\langle\xi(x,y)\rangle=0$.

The reason for the appearance of a nonspecular peak in the angular spectrum of the reflected radiation can be understood most simply by examining the scattering process in the limit of a slightly rough surface. In first-order perturbation theory in the height of the roughness, it is a simple matter to derive the following expression for the differential backscattering coefficient:

$$R(\zeta,\ \zeta_0,\varphi)=\frac{1}{(2\pi)^2}\,|\epsilon-1|^2k^4\,|E(z=0)|^2\,|E_0(z=0)|^2\,\chi(|\mathbf{k}_{0\parallel}-\mathbf{k}_\parallel|),\tag{1}$$

where ζ_0 and ζ are the glancing angles of the incident and scattered waves, φ is the azimuthal scattering angle, ϵ is the dielectric constant of the medium, and $|E_0(z)|^2$ and $|E(z)|^2$ are the spatial distributions of the field intensity in the incident and scattered waves. Far from the interface, we have[9]

$$E_0(\mathbf{r})=E_0(z)e^{i\mathbf{k}_{0\parallel}\vec{\rho}},\quad E_0(z)=\begin{cases}e^{ik_{0z}z}+Be^{-ik_{0z}z}, & z\to-\infty\\ Ae^{i\kappa_0 z}, & z\to+\infty\end{cases},$$

where $k_{0z}^2=k^2-k_{0\parallel}^2$; $\kappa_0^2=k^2\epsilon-k_{0\parallel}^2$; $k_{0\parallel}=k\cos\zeta_0$; $k=2\pi/\lambda$; λ is the wavelength in vacuum; $E(\mathbf{r})$ differs from $E_0(\mathbf{r})$ in that ζ_0 is replaced by ζ; and $\chi(q)$ in (1) is the two-dimensional Fourier transform of the correlation function of the surface roughness heights: $\chi(|\vec{\rho}_1-\vec{\rho}_2|)=\langle\xi(\vec{\rho}_1)\xi(\vec{\rho}_2)\rangle$. The reader is referred to Ref. 10 for a generalization of expression (1) which incorporates the polarization of the waves.

According to (1), the backscattering coefficient R is proportional to the intensities of the incident and scattered waves at the vacuum-medium interface and to the cross section for the scattering from one wave into the other, $\chi(q)$. At glancing angles close to the critical angle, the distribution of the wave field, $E(z)$, has the following properties[11]: When the glancing angle ζ is close to the total external reflection, ζ_c, and antinode of the wave field $|E(z)|^2$ is at the interface $(z=0)$. When ζ deviates from ζ_c, the $|E(z)|^2$ antinode moves away from the surface into vacuum, and the field amplitude at the interface, $|E(z=0)|^2$, decreases (Fig. 1). Incorporating the spread of the vacuum-medium interface in second-order perturbation theory in the roughness heights shifts the position of the maximum of the field amplitude at the surface, $|E(z=0)|^2$, into the region of glancing angles smaller than ζ_c.

Interestingly, a similar situation arises in the Bragg diffraction of x rays in crys-

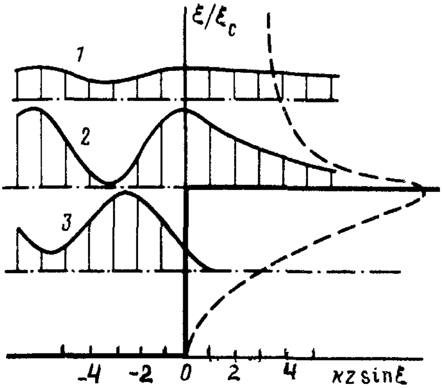

FIG. 1. Spatial distribution of the intensity of the wave field, $|E(z)|^2$, for various glancing angles: $1 - \zeta = 1.5\ \zeta_c$; $2 - \zeta = 1.0\ \zeta_c$; $3 - \zeta = 0.5\ \zeta_c$. The dashed line shows the field intensity at the surface, $|E(z=0)|^2$, versus the glancing angle ζ. The "potential" wall shows the profile of the quantity $\sqrt{1 - \mathrm{Re}\,\epsilon(z)}/\zeta_c$ along the coordinate running normal to the surface, z. Here $\zeta_c = 0.38°$ $(6.3 \times 10^{-3}$ rad); the absorption coefficient is $\nu = 470$ cm^{-1}; and the wavelength is $\lambda = 1.66$ Å.

tals, where x-ray standing waves with a period on the order of interatomic dimensions arise because of a pronounced spatial redistribution of the wave field.[12]

3. The angular distribution of the scattered radiation described by (1) has two maxima. One of them, at $\zeta \approx \zeta_0$, describes a diffuse background near the specularly reflected component of the radiation. It stems from a peak in the spectral density of the surface irregularities, $\chi(q)$, at $q = 0$ (the "forward"-scattering cross section). The value of R at $\zeta \approx \zeta_0$ is determined primarily by the scattering by large-scale irregularities. The second maximum—a nonspecular maximum—in the angular spectrum in (1) is formed on the $\chi(q)$ wing. It stems from an antinode of the intensity of the scattered wave at the surface, $|E(z=0)|^2$, at angles $\zeta \approx \zeta_c$ (Fig. 1). Since the value of R at $\zeta \approx \zeta_c$ is proportional to the spectral component $\chi(|\mathbf{k}_{0\|} - \mathbf{k}_{\|}|)$, it is clear that the anomalous peak stems from scattering by relatively small irregularities, with longitudinal dimensions on the order of $|\mathbf{k}_{0\|} - \mathbf{k}_{\|}|^{-1} \sim \lambda/\zeta_c^2$ (we are assuming $\zeta_0 - \zeta_c \sim \zeta_c$).

We wish to stress that each of the maxima in the angular spectrum arises as a result of a scattering of surface irregularities of a distinct scale. In order to simulta-

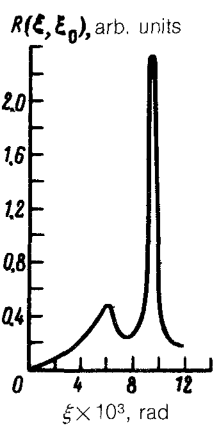

FIG. 2. Angular spectrum of the reflected radiation, $R(\zeta,\zeta_0)$, integrated over the azimuthal angle φ. The calculations were carried out with a three scale correlation function $\chi(\rho) = \chi_0 \Sigma_{i=1}^{3} a_i \exp(-\rho^2/b_i^2)$, where $a_1 = 0.1$, $b_1 = 30\ \mu$m; $a_2 = 0.1$, $b_2 = 7\ \mu$m; and $a_3 = 0.8$, $b_3 = 0.5\ \mu$m. The correlation function was taken from Ref. 14.

neously analyze the specular and anomalous peaks, we thus need information on the behavior of the correlation function of the heights, $\chi(\rho)$, over a broad range of ρ. The single-scale Gaussian model[7-9] which is ordinarily used in calculations in not suitable for this purpose, since it ignores the relatively small irregularities, and it does not permit an adequate description of the angular distribution of the scattered radiation far from the specular peak (i.e., in the "wings" of the angular spectrum). In order to describe the anomalous reflection, it is necessary to use a multiscale model and to write $\chi(\rho)$ as a set of Gaussian correlation functions with parameter values determined from independent experiments.[13,14] Figure 2 shows the results of a calculation of the angular spectrum $R(\zeta,\zeta_0)$ in a multiscale model.

The features of the backscattering of waves by an irregular solid surface which we have been discussing here are quite general in nature. They should be manifested near the critical angle in the reflection of not only photons in the x-ray range but also light, acoustic waves, neutrons, and charged particles from interfaces.

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