Dynamic effects in diffuse x-ray scattering by multilayer structures

A. V. Andreev and Yu. V. Ponomarev
Physics Faculty, M. V. Lomonosov Moscow State University, 119899 Moscow, Russia

(Submitted 17 November 1994)
Pis'ma Zh. Eksp. Teor. Fiz. **60**, No. 12, 857–860 (25 December 1994)

Effects stemming from a diffraction of waves excited by both incident and scattered waves have been observed experimentally. These effects include the emergence of forbidden reflections in the diffuse-scattering spectrum and the onset of diffuse-scattering peaks corresponding to scattering in the interior of a sample. © *1994 American Institute of Physics.*

1. In this letter we are reporting a study of how dynamic-diffraction effects help shape the angular distributions of diffuse scattering in multilayer structures. We have experimentally observed phenomena which cannot be explained by the kinematic theory of diffraction and which stem from the excitation of strong diffracted waves excited by both incident and scattered waves: Dynamic-diffraction effects lead to a strong dependence of the diffusion-scattering profile on the angle of incidence of the wave in the Bragg-reflection region, to the emergence of forbidden reflections in the diffuse-scattering spectrum, and to the onset of diffuse-scattering peaks corresponding to resonant scattering in the interior of a sample.

The angular distribution of the diffuse scattering of x radiation with a wavelength on the order of 1 Å from multilayer structures with periods ranging from a few nanometers to tens of nanometers is a few degrees wide. The size of the coherently illuminated region is thus on the order of a few centimeters, so one can work from angular distributions of the scattering to determine statistical characteristics of irregularities at the interfaces. Angular distributions of diffuse scattering were derived theoretically in Refs. 1 and 2. There has recently been extensive experimental research on diffusion scattering by multilayer structures.[3–6] Kinematic models which ignore the presence of specular components for the incident and scattered waves have been used to determine the statistical characteristics of irregularities of interfaces from experimental spectra. The present study has demonstrated experimentally that dynamic effects lead to qualitative changes in the profile of the angular distributions of diffuse scattering.

2. In the experiments we used multilayer x-ray mirrors fabricated at the Institute of the Physics of Microstructures of the Russian Academy of Sciences in Nizhniĭ Novgorod. The mirrors had periods of 30–180 Å, various pairs of materials, and various numbers of layers. The ratio of the thickness of the layer of the denser material (a) to the period (d) in the test samples lay in the range $\beta = a/d = 0.1–0.5$.

Figure 1 is a schematic diagram of the experiment. The experiments were carried out on a spectrometer with monochromatized [Ge (220)] radiation from an x-ray tube with a copper anode. The angular divergence of the radiation incident on the sample was 20″.

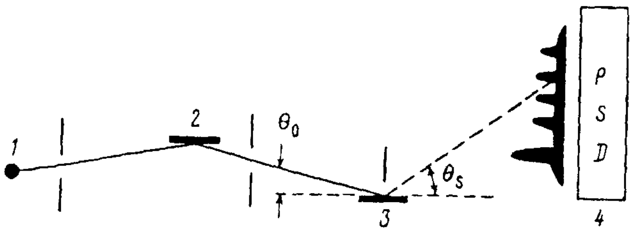

FIG. 1. Experimental layout. 1—X-ray tube; 2—monochromator; 3—test sample; 4—x-ray coordinate detector.

The scattering from the sample was detected by an x-ray coordinate detector with a 50 $\times 8$-mm^2 window and a spatial resolution of 0.2 mm.

3. Figure 2 shows experimental panoramic angular distributions of the diffuse scattering. The independent variable is the angular deviation $(\theta_0-\theta_B)$ of the incident wave from the position of the first Bragg peak. Results are shown for two multilayer mirrors: S1-24 (Fig. 2a) and S-258 (Fig. 2b). Mirror S-258 consisted of $N=17$ pairs of Mo/B_4C layers with a period $d=70.8$ Å $(\beta=0.4)$, deposited on a glass substrate. The values of the Bragg-reflection coefficients for this mirror were $R_1=75\%$, $R_2=15\%$, $R_3=16\%$, and $R_4=0.1\%$ at the wavelength of the Cu Kα_1 line. Mirror S1-24 had

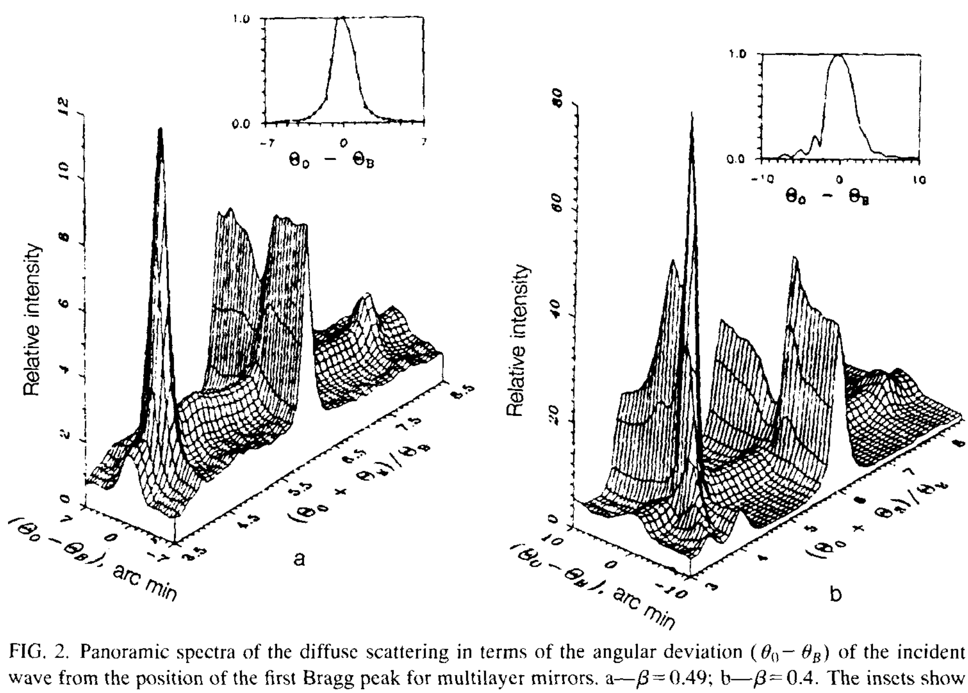

FIG. 2. Panoramic spectra of the diffuse scattering in terms of the angular deviation $(\theta_0-\theta_B)$ of the incident wave from the position of the first Bragg peak for multilayer mirrors. a—$\beta=0.49$; b—$\beta=0.4$. The insets show the intensity (I) of the specular component versus the angular deviation from the first Bragg peak.

$N=35$ Fe/C layer pairs with a period $d=51.8$ Å ($\beta=0.49$) on a silicon substrate. Its reflection coefficients were $R_1=55\%$, $R_2=0.05\%$, and $R_3=1.1\%$ at the Cu $K\alpha_1$ line.

Along with the nonresonant background in the angular distribution (Fig. 2) we can see some peaks of resonant diffuse scattering. In a first approximation the positions of these peaks are described by $\theta_0+\theta_S=2n\theta_B$, where n is the order of the peak. If the angle of incidence of the x radiation is far from the Bragg-reflection region, $|\theta_0-\theta_B|\gg\Delta\theta_B$ ($\Delta\theta_B$ is the width of the Bragg-reflection region), then the parameters (height and width) of the peak of resonant diffuse scattering are determined by statistical characteristics of the interfaces (the mean square roughness height and the longitudinal and transverse correlation lengths)[1] and the corresponding Fourier component of the polarizability. The insets in Fig. 2 show the intensity of the specular component versus the angular deviation. These plots give an idea of the width of the region of the first Bragg reflection. We see from Fig. 2a that outside the Bragg-reflection region there is a clearly defined third diffuse resonant peak. The peaks of even orders are essentially suppressed because of a selection rule in terms of the structure factor $f_h=1-\exp(i\,\mathbf{H}ha)$ ($\mathbf{H}=2\pi/d$ is a reciprocal-lattice vector).

In the Bragg-reflection region in terms of the incident wave, the angular distribution changes qualitatively: The intensity of the nonresonant background increases, the intensities of the resonant peaks become strongly dependent on the angular deviation, and the intensities of "forbidden" resonant peaks increase sharply (Fig. 2a). These changes stem from the onset of a system of coupled x-ray standing waves, which are formed by both the incident wave and the diffusely scattered waves, and also from changes in the phases of these interference fields. By varying the angle of incidence we can vary the position of the antinodes of the interference fields with respect to the interfaces. We can thus determine both the average profile of the interfaces and the statistical characteristics of the interfaces more accurately. The reason for the increase in the intensity of the nonresonant background is an increase in the extinction length in the Bragg-reflection region. The extinction length determines the formation of the scattered radiation. In a first approximation, if we ignore the effect of the interference field of the scattered waves, the intensification of the "forbidden" resonant-scattering peaks occurs because the formation of the peaks is forbidden in terms of the structure factor for the incident wave, while it is allowed in terms of the structure factor for the diffracted wave. The behavior of the intensities of the resonant peaks as a function of the angular deviation is governed by the interference fields caused by both the incident waves.

The formation of resonant peaks in the Bragg-reflection region is determined by dynamic effects involving both the incident wave and the reflected and scattered waves, as follows from the panoramic angular distribution of the diffuse scattering for the mirror with $\beta=0.4$ (Fig. 2b). This spectrum has two peaks at negative angular deviations in the region $\theta_0+\theta_S=4\theta_B$. This structure is evidence of a resonant excitation of scattered waves at two branches of the dispersion surface in relatively thin multilayer structures. The interference of these waves also explains the double-hump structure of the peak in the resonant diffuse scattering as a function of the angular deviation. The experimental detection of the additional peak, with a smaller exit angle θ_S, indicates that the kinematic approach which is ordinarily used is incomplete, and that dynamic diffraction of scattered waves must be taken into account in the consideration of the formation of the scattered field.

4. These experiments clearly demonstrate that the kinematic diffraction theory often does not yield a correct description of the angular distributions of diffuse scattering by multilayer structures. Dynamic-diffraction effects (involving both the incident wave and the scattered waves) lead to qualitative changes in the angular distributions of the scattering: to the emergence of forbidden reflections and to the onset of additional peaks in the resonant scattering. Research on the angular distributions of the diffuse-scattering spectra in the region of dynamic diffraction in terms of the incident wave will add substantially to our ability to reconstruct the average profile of the density of multilayer structures and to determine statistical characteristics of interfaces between layers.

We wish to thank N. N. Salashchenko and Yu. Ya. Platonova for furnishing the multilayer x-ray mirrors and for a discussion of the results.

[1] A. V. Andreev *et al.*, J. Mod. Phys. **35**, 1667 (1988).
[2] V. Holy *et al.*, Phys. Rev. B **47**, 15896 (1993).
[3] D. K. G. de Boer *et al.*, Appl. Phys. A **58**, 169 (1994).
[4] V. Holy and T. Baumbach, Phys. Rev. B **49**, 10688 (1994).
[5] V. Pietsch *et al.*, Thin Solid Films **247**, 230 (1994).
[6] T. Salditt *et al.*, *Programme and Abstracts of 2nd European Symposium on X-ray Topography and High Resolution Diffraction* (Humbolt Univ., Berlin, 1994), p. 23.

Translated by D. Parsons