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Si/SiO_2 interface-depth determination in glancing-incidence X-ray diffraction experiments.

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Abstract

The Si/SiO_2 interface of a single crystal has been investigated by the double-crystal inclination method, the surface peak being measured. The distorted layer depth is shown to be of the order of 1 nm and the amorphous film depth of the order of 6 nm.

In the first experiments on glancing-incidence diffraction by Marra, Eisenberger & Cho (1979), it was shown that the Laue diffraction-surface sensitivity is considerably enhanced. However, the geometry of these experiments suggests a rather high collimation with respect to both the glancing angle Φ_o and the deviation angle from the Bragg condition $\Delta\theta$. The $\Delta\theta$-collimation difficulties are overcome in the scheme suggested by Afanas'ev & Melkonyan (1983) and by Imamov, Golovin, Stepanov & Afanas'ev (1983), which is based on the relationship between the incident angle Φ_o and the exit angle Φ_h:

$$\Phi_h^2 = (\Phi_o + 2\varphi \sin\theta_B)^2 + \alpha, \quad \alpha = 2\Delta\theta \sin 2\theta_B, \qquad (1)$$

where φ is the misorientation angle between the diffraction planes and the surface normal and θ_B is the Bragg angle.

However, there is a real advantage in dealing with the diffraction intensity as a function of Φ_o at fixed α, owing to the rotation around the inverse lattice vector **H** [the so-called inclination method, proposed by Somenkov, Schilstein, Belova & Utemisov (1978)].

Total reflection is always accompanied by an enhancement factor,

$$|2\Phi_o/\Phi_o + (\Phi_o + \chi_o)^{1/2}|^2, \qquad (2)$$

where χ_o is the media polarizability. In the case of X-ray diffraction, the resulting signal is also enhanced by the factor

$$|2\Phi_h/\Phi_h + (\Phi_h^2 + \chi_o)^{1/2}|^2. \qquad (3)$$

Considering the diffraction intensity as a three-dimensional surface over the (α, Φ_o) plane, one can find the following ridges for rather large values of $|\alpha|$:

$$\begin{aligned} &\Phi_o = \Phi_c \text{ at } \alpha \gg \Phi_c^2, \quad \text{from (2);} \\ &\Phi_h = \Phi_c \text{ at } -\alpha \gg \Phi_c^2, \quad \text{from (3);} \\ \text{or} \quad &\Phi_{o\alpha-} = -2\varphi \sin\theta_B - (-\alpha + \Phi_c^2)^{1/2} > 0 \quad \text{and} \\ &\Phi_{o\alpha+} = -2\varphi \sin\theta_B + (-\alpha + \Phi_c^2)^{1/2} > 0, \quad \text{from (1);} \end{aligned} \qquad (4)$$

where Φ_c is the critical angle.

The diffraction intensity is negligible far from the curve $\Phi_{o\alpha+}$ for rather large negative α. On the other hand, the incident beam is collimated with respect to α in a rather narrow interval of the 'Darwin table'. So, the resulting intensity curve consists of two peaks, analogous to triple-crystal diffractometry (TCD) rocking curves. The peak at $\Phi_o = \Phi_c$ corresponds to the 'Darwin table tail' and the diffraction maximum at small α, while the peak shifting with decreasing α according to (4) is due to the diffraction intensity 'tail' at large negative α and to the narrow centre

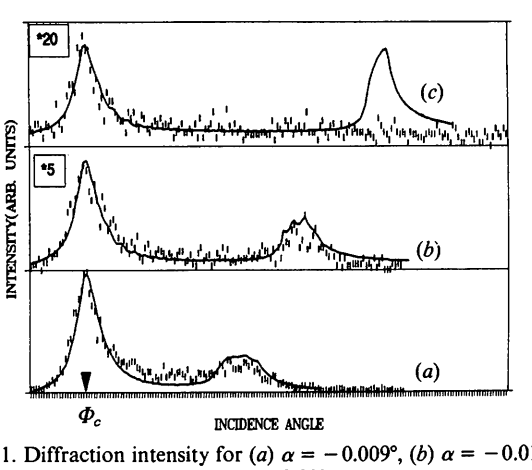

Fig. 1. Diffraction intensity for (*a*) $\alpha = -0.009°$, (*b*) $\alpha = -0.016°$, (*c*) $\alpha = -0.03°$.

of the 'Darwin table'. Hence, one can distinguish high-momentum-transfer intensity and scan it along $\Phi_{o\alpha+}$ for large negative α (Aleksandrov, Belova & Fanchenko, 1992); the peak at $\Phi_o = \Phi_c$ is the TCD-pseudopeak analogue and the peak shifting with α is the TCD-main-peak analogue.

In the case considered, the normal momentum transfer is $Q = 2\pi(\Phi_o + \Phi_h + 2\varphi \sin\theta_B)/\lambda$, so that the main-peak intensity depends on the subsurface crystal structure with characteristic depth $L \simeq 1/Q$. Thus, the diffraction measurements provide spatial resolution of the order of

$$L_\alpha = (-\Phi_c^2/\alpha)^{1/2}\lambda/2\pi\Phi_c. \quad (5)$$

In surface-peak observation experiments, a parallel diffraction scheme was used. The exposure time did not exceed 20 s for the standard X-ray tube with Cu $K\alpha$ radiation used. Perfect silicon single-crystal specimens were cut out parallel to the (100) surface.

The experimental diffraction curves for the 022 reflection and different values of $\Delta\theta$ are shown in Fig. 1. The theoretical curves were calculated within the framework of the usual theory (Aleksandrov, Afanas'ev, Melkonyan & Stepanov, 1984), the dispersion also being accounted for. According to (5), the spatial resolutions are about 2.1, 1.5 and 1.0 nm for the curves in Fig. 1. The disappearance of the experimental surface peak in the case of curve (*c*) may be explained by the presence of the distorted Si/SiO_2 interface, its depth being of the order of 1 nm according to data from Feldman, Salverman, Williams, Jackman & Stensgaard (1978).

The Si/SiO_2 amorphous-film depth may be obtained from the form of the zero-angle front of the TCD-pseudopeak-analogue curve. In the case considered, the amorphous-film depth was about 6 nm.

For a more detailed investigation, some model of the interface structure should be taken into account. Without it, only the model-independent depth can be reconstructed. Nevertheless, the inclination method proved to be very useful in surface-structure study.

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