

Modulation of the Amorphous Structure of SiO₂ on Si(001)

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Introduction

Thin films of SiO₂ are widely used as gate oxides in Si-based integrated circuits [1]. One reason for the technological success of this material combination is the extraordinary flat and reliable interface of the amorphous SiO₂ in contact with the perfectly crystalline Si. Numerous experimental and theoretical investigations have described particular features of this interface. X-ray reflectivity [2] as well as photoelectron spectroscopy [3] and electron energy loss spectroscopy [4] experiments have suggested the existence of an intermediate or interfacial layer between the amorphous SiO₂ and the silicon substrate. Although there is an extensive amount of literature on scattering from bulk silica glass, no measurement of the amorphous structure factor of thin (100 Å) SiO₂ layers has been reported so far. We present measurements of the amorphous structure factor of a 100-Å SiO₂ layer on Si(001) by using grazing incidence diffraction (GID).

If we consider a continuous random network of SiO₄ tetrahedra, the resulting scattering distribution consists of several broad maxima corresponding to structural correlations in the glass. A strong peak at 1.5 Å⁻¹ is usually referred to as the first sharp diffraction peak (FSDP). As pointed out by Moss and Price [5], the FSDP is associated with medium-range correlations in the glass; namely, the mean distance between SiO₄ structural units. The FSDP in bulk glass, as with all other diffraction features, is perfectly isotropic in real and reciprocal space, resulting in smooth haloes of scattering intensity.

Methods and Materials

The samples under investigation were prepared by using dry oxidation in a furnace; no attempts were made to remove the natural oxide. The 100-Å sample was oxidized at 800°C. During the measurements, the sample was enclosed in a Be can under protective helium atmosphere. The x-ray energy was 20 keV, resulting in a critical angle for total external reflection for the SiO₂ of 0.08°. GID scans were accomplished by inclining a vertical diffractometer with respect to the incident beam and collecting the diffracted photons with a scintillation counter with an open slit in the direction perpendicular to the sample surface. The resulting scattering depth sampled the entire thickness of the SiO₂ layer.

Results

Figure 1 shows the scattering distribution in the {hk0}-plane of the sample at an incident angle of 0.05°. The diffuse ring corresponding to the FSDP is modulated at the positions of the Si(110) reflections, which are themselves forbidden by symmetry. It should be clearly noted that there is no harmonic contamination at these positions as determined experimentally by using beam attenuators. The upper part of Fig. 1 shows a single phi scan at the position of the Si(110) reflection (i.e., at 1.636 Å⁻¹). The modulation is fourfold, with a width of several degrees, and the entire ring is not circular (i.e., the position of enhanced intensity along [110] occurs at 1.6 Å⁻¹, while the remainder occurs closer to 1.4 Å⁻¹). Since the enhanced FSDP of our sample coincides with the Si(110) position, we calculate a concomitant compression of the structural units of the SiO₂ by about 8% in this direction.

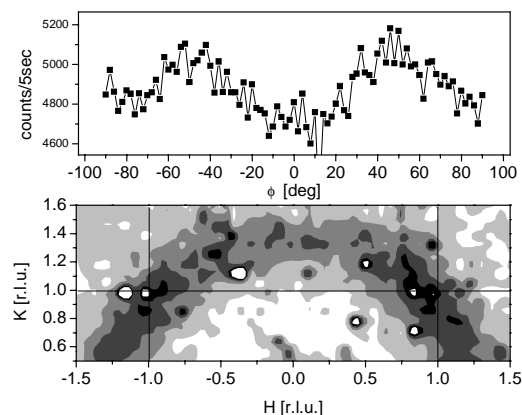


FIG. 1. Scattering distribution in the {hk0}-plane of the sample at an incident angle of 0.05°.

Discussion

As demonstrated through an analysis of the partial structure factors of a relaxed Bell and Dean model [6], there are at least three correlations and their multiples contributing to the FSDP. We have highlighted these contributions in our proposed model of the *local* structure

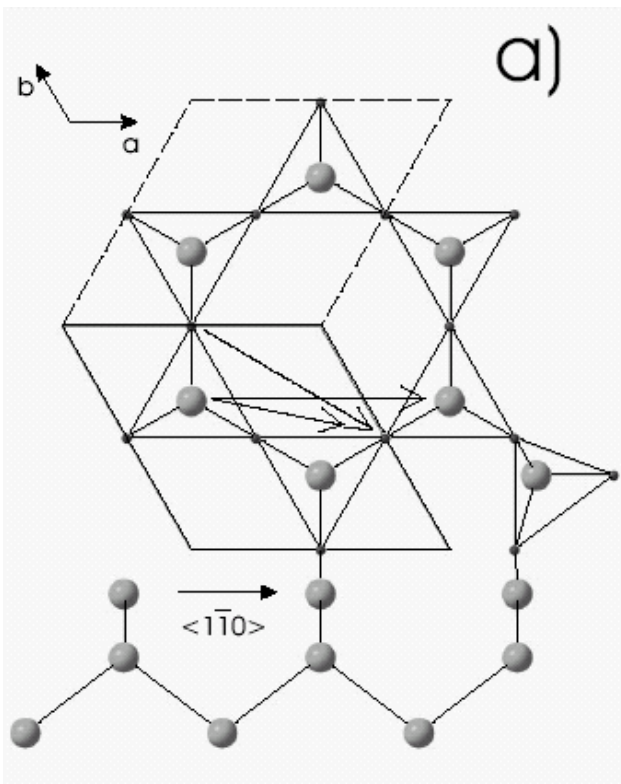


FIG. 2. Proposed model of the local structure near the interface.

near the interface (arrows in Fig. 2). Since, according to our observations, the Si(110) directions enhance the FSDP correlations, it is likely that zig-zag chains of corner-sharing tetrahedra are located near the interface. Thus there is a certain probability that these random zig-zag chains “freeze” into a tridymite-like structure.

Acknowledgments

Use of the APS was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. W-31-109-ENG-38. We thank J. Lang for assistance and R. Nemanich for the sample preparation.

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