Use of Thin Si Crystals in Backscattering-Channeling Studies of the Si-SiO$_2$ Interface

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We report on new information obtained on the nature of the nonregistered Si layers at the Si-SiO$_2$ interface using MeV backscattering-channeling techniques on thin Si single crystals. Analysis of the scattering intensity from the front and back surfaces of the crystal allows us to conclude that the atoms in the nonregistered monolayers have a displacement from the "bulk" position between 0.1 and 1.0 Å.

Recent investigations of the Si-SiO$_2$ interface by MeV backscattering-channeling techniques have indicated that the oxide is stoichiometric SiO$_2$ to within a few angstroms of the substrate and that the first monolayers of the silicon crystal are not registered, that is, do not retain the bulk structure.[1] In that study, we measured the Si ⟨110⟩ surface peak and oxygen peak of thick (110) crystals using an emergent grazing-angle geometry (detector at ~94° scattering angle). When plotted on a Si-vs-O curve the data were extremely well fitted by a straight line corresponding to SiO$_2$ plus an additional 8.8×10^{15} Si/cm^2. Since the calculated surface peak from an ideal unreconstructed Si single crystal in this case is 6.4×10^{15} Si/cm^2, the extra 2.4×10^{15} Si/cm^2 is the equivalent of ~2 nonregistered layers of Si under the oxide. (We could not distinguish between one nonregistered layer plus ~5 Å of SiO and simply two nonregistered layers and SiO$_2$.) From these measurements alone the structural nature of these layers could not be determined; the results are consistent with an amorphous structure, a reconstructed ordered layer, or a random array of atoms displaced >0.15 Å. In this Letter we report on further aspects of this study making use of thin Si single crystals. We obtain significant new information on the structure of the nonregistered layers, confirm the stoichiometry of the oxide, and illustrate, for the first time, the unique advantages of the thin-crystal technique for this type of study.

The nature of the backscattering spectra recorded from an aligned thin crystal is shown schematically in Fig. 1(a). As a result of finite resolution, the Si front-surface peak Si(*F*) combines contributions from the Si in the oxide, from nonregistered Si at the interface, and from the first monolayers of the single crystal. This latter contribution, denoted the intrinsic surface peak, corresponds to the surface peak intensity that would be observed from an ideal single crystal terminated at the surface with the bulk structure. Since the first monolayer(s) of the single crystal is exposed to the uniform flux distribution of the incident beam, the intrinsic surface peak will correspond to scattering from at least one monolayer. Additional monolayers will contribute depending on the vibration amplitudes of the

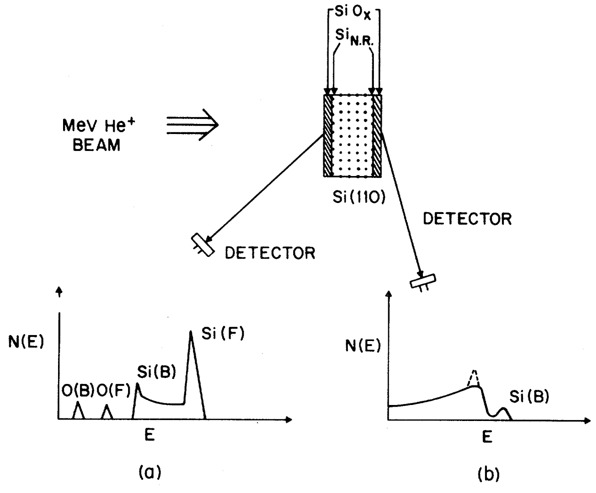

FIG. 1. Schematic of the aligned backscattering spectrum observed in two different geometries: (a) ~170° scattering angle; (b) ~84° scattering angle; the position of the surface peak in the absence of anomalous energy loss is indicated by the dashed line. SiO$_x$ refers to the oxide, Si$_{\text{N.R.}}$ refers to the nonregistered Si.

atoms in the crystal and the scattering parameters of the atomic system. The intrinsic surface peak has been studied in detail recently, both experimentally and theoretically, for surface physics applications.[2]

As the beam penetrates deeper into the crystal (~500 Å) the flux distribution is modified by the channeling process; only a small portion (~3%) of the beam is available for large-angle scattering while the channeled component (~97%) has a flux distribution sharply peaked at the channel center. At the crystal back surface, the channeled beam may interact only with the nonregistered layers (depending on their displacement) and with the amorphous oxide, giving rise to a back-surface peak of Si, Si(*B*). The first monolayers(s) of an ideal single crystal make almost no contribution to the scattering on the exit side since the channeled beam has no intensity at the normal lattice sites on the back surface. Thus, the difference in intensity of the front- and back-surface peaks is given by the intrinsic contribution and a contribution depending on the number and displacement of the nonregistered layers; nonregistered layers which are amorphous (random) would contribute equally to both the front- and back-surface peaks.

At lower energies in the spectrum the front- and back-surface oxygen peaks are visible. An experimental spectrum for 1.2-MeV He^+ scattering from a 1700-Å Si crystal is shown in Fig. 2. As shown, the areas of the two oxygen peaks are approximately equal indicating that the oxide thickness is approximately the same on both surfaces. The Si surface peaks have a large difference in magnitude since the intrinsic contribution is dominant in the front-surface peak. Since structural information is often contained in the difference between the measured surface peak and that calculated from an ideal crystal, it can be seen that the back-surface peak is the more sensitive measure of displacements.

It is difficult, however, to extract the area of the back-surface peak precisely (in Fig. 2) since the background is not well understood. This problem may be overcome by observing the spectrum in a transmission grazing-angle geometry, as shown schematically in Fig. 1(b). In this geometry, the scattering occurring at the back surface now becomes the leading edge of the spectrum since those particles have traveled the shortest path through the crystal. The crucial advantage of this technique arises from the anomalously low energy loss of the channeled component of the beam; thus, the exit-surface peak associated with the interaction of the channeled beam with the oxide and displaced Si on the back occurs at higher energy, removing it from the background associated with the nonchanneled component. This effect results in a more easily analyzed silicon surface peak.

A comparison of the transmission grazing-angle spectra from a silicon sample (~7000 Å) with ~17 Å of native oxide in a channeling and nonchanneling direction is shown in Fig. 3. The Si back-surface peak displaced to higher energy

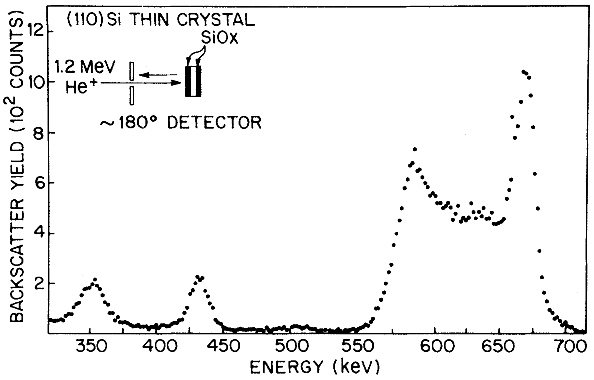

FIG. 2. The backscattering spectrum for the geometry indicated by (a) in Fig. 1. The various peaks are discussed in the text.

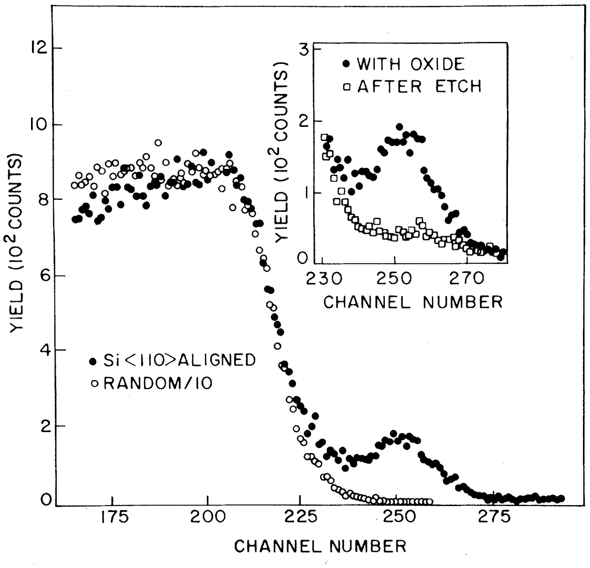

FIG. 3. Spectra taken in the geometry indicated in Fig. 1(b): ○, nonaligned spectra; •, aligned spectra. The inset shows two aligned spectra: •, with ~18 Å of oxide, and □, with less than 3 Å of oxide.

is clearly shown in the aligned spectrum. The difference between the peak position and the leading edge of the nonchanneling spectrum is determined by $kt\,|(dE/dx)_R - (dE/dx)_C|$ where k is the kinematical factor, t is the crystal thickness, and $(dE/dx)_R$ and $(dE/dx)_C$ are the random and channeled stopping powers, respectively. The lack of perfect separation between the peak and the continuum undoubtedly occurs because of a spread in $(dE/dx)_C$ associated with different channeling trajectories. The inset in Fig. 3 compares the area of the back-surface peak before and after a HF etch to remove the oxide. The area of the oxygen peaks in each case was determined in a backscattering grazing-angle geometry described in detail elsewhere.[1] The absolute areas of the oxygen and silicon peaks were determined using a Bi-implanted silicon standard.

The numerical results, after corrections for energy-loss effects and channeled beam intensity,[3] are condensed in Table I. Note that the oxide removed during the etch was very close to being SiO_2 as was found earlier. Upon comparing the silicon-surface-peak areas (front and back), we note differences of 9.5×10^{15} Si/cm^2 and 9.9×10^{15} Si/cm^2 for the oxidized and etched cases, respectively. For this energy, 1.2-MeV He^+, the intrinsic surface peak value is 7.8×10^{15} atoms/cm^2, yielding differences of 1.7×10^{15} and 2.1×10^{15} atoms/cm^2. This implies that the ~2 extra monolayers of nonregistered Si previously reported as contributing to Si(F) do not contribute to Si(B).

A likely explanation of this difference lies in the magnitude of the atomic displacements of the nonregistered monolayers. Figure 4 shows the sensitivity to displacement for contributions to the front-surface peak and the back-surface peak. Since the channeling flux is so strongly concentrated at the channel center, large atomic displacements, ~1 Å, are required in order to give a substantial contribution to the Si(B) yield. The front-surface peak sensitivity is dominated by the shadow cone radius and requires displacements of only ~0.1 Å. [In principle, one can reduce the range of limits set here by measuring Si(B) as a function of tilt from the aligned direction. However, further measurements on the energy-loss distribution as a function of incident angle are required to make quantitative use of this important refinement.] The picture of the interface which now emerges from the measurements is the following: The oxide is stoichiometric SiO_2 to within a few angstroms of the surface. At the interface there are 1–2 monolayers of Si which are not amorphous but have atomic displacements between 0.1 and 1 Å from the normal Si positions. Underlying those layers is the Si single-crystal substrate.

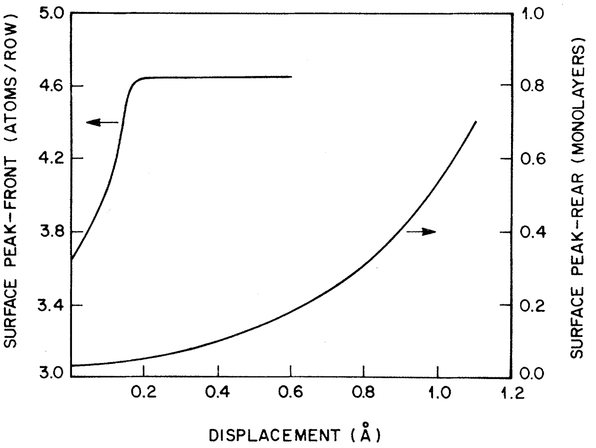

FIG. 4. Displacement sensitivity of the front- and back-surface peaks for 1.0-MeV He in Si⟨110⟩. The rear surface peak as a function of displacement from "bulk" position is extracted from Ref. 4. A normalized yield of 1.0 corresponds to one complete monolayer. The calculated surface peak (F) as a function of displacement of the first atom for 1.0-MeV He^+ on Si ⟨110⟩ is extracted from Monte Carlo simulations. Note the difference in displacement required for an increased yield of one monolayer.

TABLE I. Surface-peak and oxygen areal densities[a] (10^{15} atoms/cm^2).

	Si_{front}	Si_{back}	O
Oxide	13.8 ± 0.7	4.3 ± 0.5	7.4 ± 0.4
Etched	10.6 ± 0.5	0.7 ± 0.5	1.0 ± 0.1

[a] All of these measurements are on the same surface of the thin Si crystal. Si_{front} and Si_{back} refer to the experimental geometry, not to the two different surfaces.

We have illustrated that ion backscattering and channeling in thin crystals can yield important information on the nature of the interface. The data illustrate that the basic origins of the intrinsic surface peak in this type of experiment are well understood. There are obvious extensions to clean crystal surface and adsorbate studies.

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[1] L. C. Feldman, I. Stensgaard, P. J. Silverman, and T. E. Jackman, in Proceedings of International Conference on the Physics of SiO_2 and its Interfaces, edited by S. T. Pantelides (Pergamon, New York, to be published).

[2] I. Stensgaard, P. J. Silverman, and L. C. Feldman, to be published.

[3] By immediately placing the sample in the vacuum system ($\sim 10^{-7}$ Torr) after the HF etch the oxygen coverage can be limited to ~1 monolayer.

[4] The "channeling beam intensity correction" refers to the fact that only channeled particles contribute to the shifted back-surface peak. This correction is determined experimentally by noting, as in Fig. 3., that the minimum yield at the back surfaces is ~0.1. Thus the correction is ~10%.

[5] Part of Fig. 4 is adapted from a calculation of S. T. Picraux, W. L. Brown, and W. M. Gibson, Phys. Rev. B 6, 1382 (1972).

Monte Carlo Test of Theories for the Planar Model, the *F* Model, and Related Systems

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We have performed Monte Carlo simulations for correlation functions in various solid-on-solid models, some of which are equivalent to the *F* model, the two-dimensional Coulomb gas, and the planar model. Our results for the *F* model can be quantitatively represented using the theory of Kosterlitz and Thouless. We use this theory to help determine the transition temperatures in other systems.

Recently there have been several diverse predictions concerning the critical properties of the planar (classical XY) model[1-6] and closely related systems such as the two-dimensional Coulomb gas and various solid-on-solid (SOS) models for the interface roughening transition.[7-9] Kadanoff[10] has provided arguments suggesting that a number of other systems, including in particular the F model,[11] should have similar critical behavior. Experimental systems to which these theories are expected to apply include planar magnets[12] and liquid crystals,[13] melting of two-dimensional crystals,[2,14] the crystal-vapor interface,[7-9] and ^{4}He films.[2,15,16]

In this Letter we report Monte Carlo (MC) calculations of correlation functions in a variety of SOS models. Our results for a system equivalent to the F model can be fitted quantitatively by the theory of Kosterlitz and Thouless[2,3] (KT) and José *et al.*[6] Since extensions of the KT theory[17] have also successfully predicted the magnitude of the jump in the superfluid density at T_c for ^{4}He films,[16] it seems clearly favored over the alternative approaches. We then analyze the MC data using the KT theory to determine the transition temperatures for the other systems.

A general SOS model is characterized by a two-dimensional array of columns of varying *integer* heights h_j. In a lattice-gas picture the h_j give a measure of the number of atoms in column j. The interaction energy $V(h_j - h_{j+\delta})$ is some increasing function of the difference in heights between columns passing through nearest-neighbor sites j and $j+\delta$. A case of special interest in the theory of crystal growth,[7] denoted ASOS herein, is a square array of columns with $V_A = J|h_j - h_{j+\delta}|$. Also of interest is the discrete Gaussian model with $V_{DG} = J|h_j - h_{j+\delta}|^2$ which can be mapped exactly onto a two-dimensional Coulomb-gas system.[8] Furthermore, it has been shown[6,18] that these and other SOS models can also be mapped exactly onto a generalized planar model with an interaction energy $\tilde{V}(\theta_j - \theta_{j+\delta})$ that depends on the difference in angles between nearest-neighbor spins and with $\tilde{V}$ a simple transform of the SOS energy V.

Thus computer simulations of these various SOS models provide direct information about the phase transitions in the corresponding planar models, and in the case of the discrete Gaussian model, the Coulomb gas. The SOS representation with its discrete excitations is particularly convenient for computer simulation work. Furthermore, direct simulation of the usual planar model at low temperatures is very difficult because of the existence of frozen-in vortices.[19]

The phase transition can be characterized by the behavior of the correlation function relating