

Investigation of the Atomic Structure of the SiO₂/Si(111) Interface by MEIS (Medium-Energy Ion Scattering)

T. NISHIOKA, Y. SHINODA, C. HEIMLICH, Y. KOBAYASHI, H. HIBINO and K. SUGII*

NTT Basic Research Laboratories
Midori-cho 3-9-11, Musashino-shi, Tokyo 180

The atomic structure of the thin SiO₂/Si(111) interface was investigated by medium-energy ion scattering (MEIS). The Si crystal structure under the interface differs between a thermal oxide system and a native oxide system. The Si atoms in the thermal oxide system are displaced from their ideal lattice positions at depths up to at least 10 nm. A native oxide system, in contrast, has a relatively simple structure: the top two bilayers of the Si crystal are displaced upward toward the oxide, and there is a normal bulk crystal structure underneath.

1. Introduction

The SiO₂/Si interface has been the subject of much research related to submicron MOS process technology. Device characteristics are directly tested by measuring the interfacial electrical properties, but information on the atomic structure is clearly essential to an understanding of the interface properties. And although various techniques - including photoelectron spectroscopy,¹⁻³⁾ transmission electron microscopy (TEM),⁴⁾ infrared spectroscopy,⁵⁾ and ion scattering⁶⁾ - have been used to investigate the interfacial structure, very little is known about the atomic structure on the crystal side of the interface.

Medium-energy ion scattering (MEIS)⁷⁾ is a powerful technique for investigating surface and subsurface atomic structures with subangstrom accuracy. In fact, MEIS is more than an order of magnitude accurate than TEM. MEIS is an especially sensitive technique for evaluating the atomic displacement of the first several underlying Si layers and the crystal region to a depth of 10 nm. This paper reports MEIS analysis of the difference between the interfacial atomic structure of native-oxides/Si(111) and of thermal-oxides/Si(111). This analysis shows that the Si atoms in the thermal oxide system are displaced from their ideal crystal structure at depths of at least 10 nm.

2. Samples and MEIS Experiment

The wafers used in this work were 4-6 ohm-cm CZ p-Si(111). After RCA cleaning, the native oxide was formed by treating a wafer with hot HNO₃ for 5 min. The thermal oxide was prepared by oxidation in dry O₂ at 700°C for 5 min. Thicknesses of the oxides, evaluated by Auger electron analysis and/or ellipsometric methods, were 1.0 - 1.2 nm for the native oxide and 1.6 - 1.7 nm for the thermal oxide.

Displacement of the crystal Si atoms from their lattice positions was investigated using the double alignment (channeling/blocking) technique of MEIS.⁷⁾ One experimental geo-

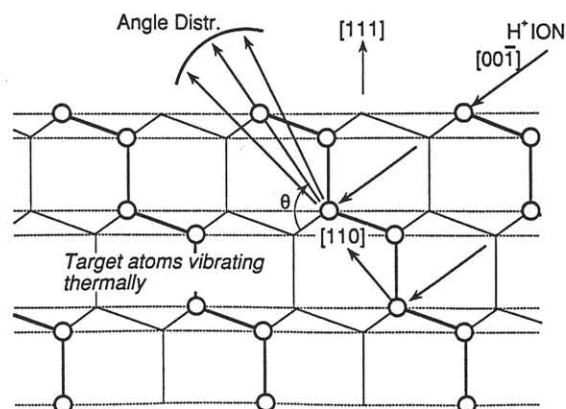


Fig. 1. Alignment geometry of channeling and blocking relative to a Si crystal.

*Present address: NTT Opto-electronics Laboratories, Tokai, Naka-gun, Ibaraki 319-11.

metry is shown in Fig. 1; 100-keV H^+ ions are incident along $[00\bar{1}]$ and scatter around $[110]$. Some of the scattered ions are shaded, for example, by the atoms in the first layer, resulting in a dip in the angle distribution. A toroidal shaped electrostatic analyser⁷⁾ able to measure scattered ion intensities within an arc of 25° was placed so that the measured arc included the $[110]$ direction. Figure 2 shows one set of data obtained through MEIS. The ion yield is a function of the scattering angle and the energy of the scattered ion. The energy axis is related to depth information, which is the same as in the normal Rutherford backscattering technique. By adding the scattering yields within a specific small energy window (that is, at a specific depth), we can acquire an

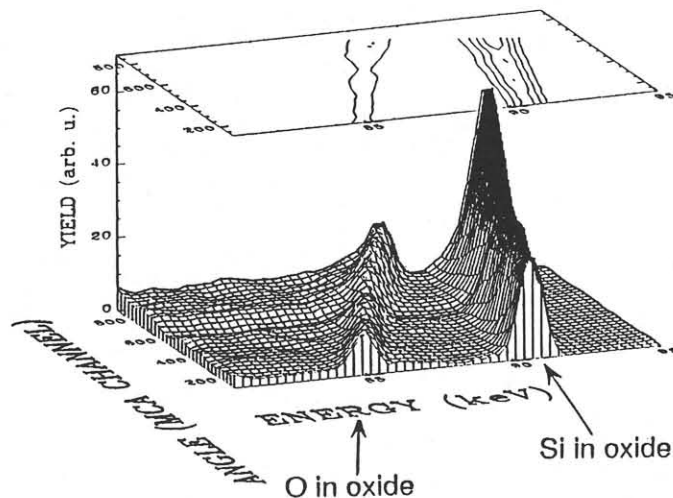
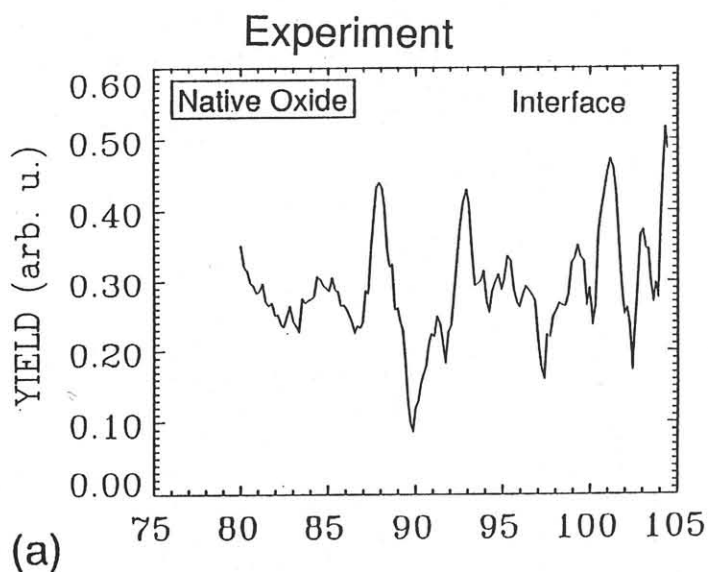
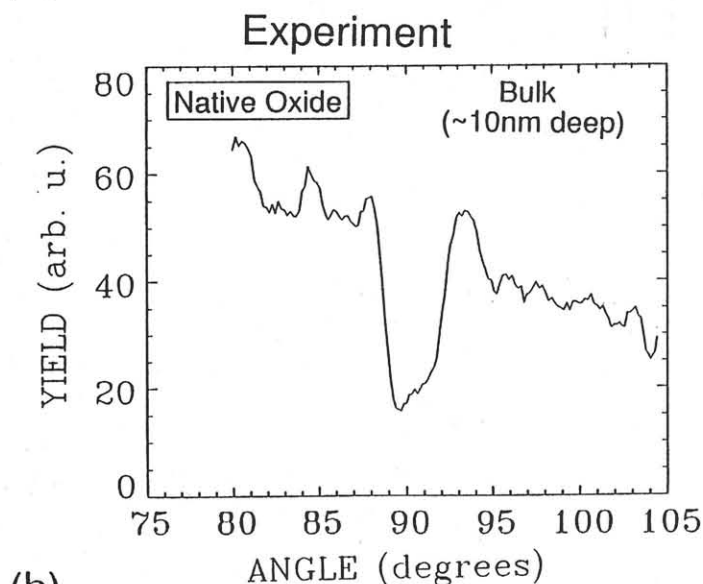


Fig. 2. An example of data obtained through MEIS.



(a)



(b)

Fig. 3. Angle spectra of a native oxide system from (a) a near-interface region, and (b) a bulk-crystal region.

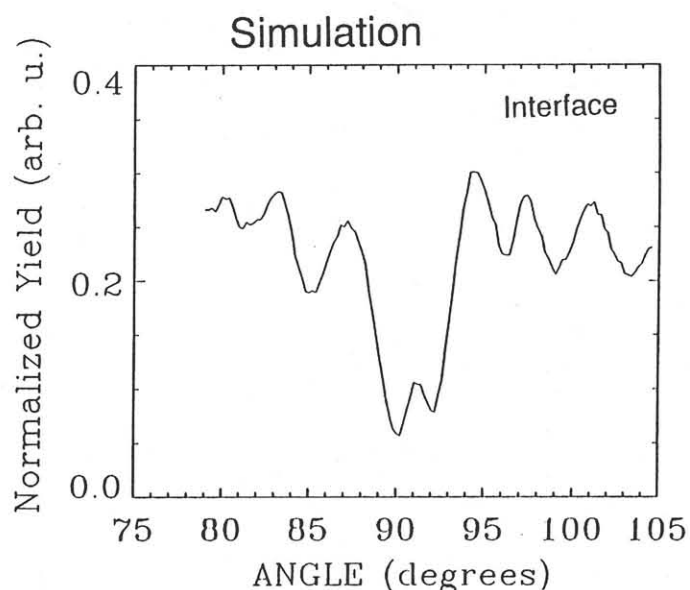


Fig. 4. A Monte Carlo simulation of ion scattering in the near-interface region.

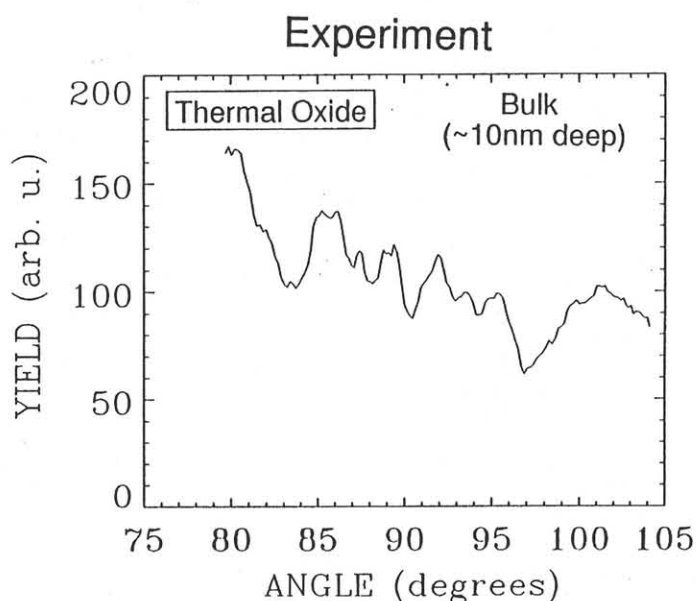


Fig. 6. Angle spectrum of a bulk-crystal region in a thermal oxide system.

angle distribution originated from the corresponding depth of the sample.

In this work, we used the geometries of [111]- and $[\bar{1}\bar{1}\bar{1}]$ -scattering, as well as [110]-scattering. Combining the angle distribution results of these 3 geometries gives information on the 3-dimensional atomic structure at various depths of the interface and/or underlying crystal.

3. Results and Discussion

Figures 3 shows angle spectra of ion yields from a near-interface region and from a bulk-crystal region (about 10 nm deep) in the native oxide system. While the angle spectrum of the bulk crystal has a large blocking dip at 90° , the spectrum of the interface has a split dip near 90° and several smaller dips.

To determine the Si structure of the native oxide system, Monte Carlo simulation of ion scattering⁸⁾ was performed. The bulk spectrum shown in Fig.3(b) agrees well with a simulation result based on the ideal Si crystal structure. The results obtained with the [111]-scattering (sample normal direction) geometry, where only the lateral displacement affects the angle distribution, showed that the lateral displacement near the interface was small ($<0.01\text{nm}$). We can therefore consider only vertical displacement in the simulation. One of the results from the simulation of the near-interface region is shown in Fig. 4, which shows the same characteristic profile as the experimental interface spectrum shown in Fig. 3(a). Although these profiles are not fully matched (because an overlayer corresponding to the oxide was omitted from the simulation), the positions of the blocking dips are very similar in these two figures. Figure 5 shows the structure model used in this simulation; the two top bilayers of Si are displaced upward toward the oxide.

A bulk angle spectrum of the thermal oxide system, which differs from the spectrum of the native oxide system (Fig.3(b)), is shown in Fig. 6. From just under the oxide to more than 10 nm deep in the thermal oxide system, the Si atoms proved to be displaced from the ideal crystal structure.

This specific blocking pattern cannot be explained by the ideal bulk-crystal structure. The native oxide system, in contrast, has a relatively simple structure as described above. It should be noted that Si atoms in the thermal oxide system are displaced from their lattice positions even at a depth of 10 nm. MOS electron conduction characteristics have conventionally been discussed on the basis of an ideal crystal structure, but the discovery of this displacement may require a new approach to

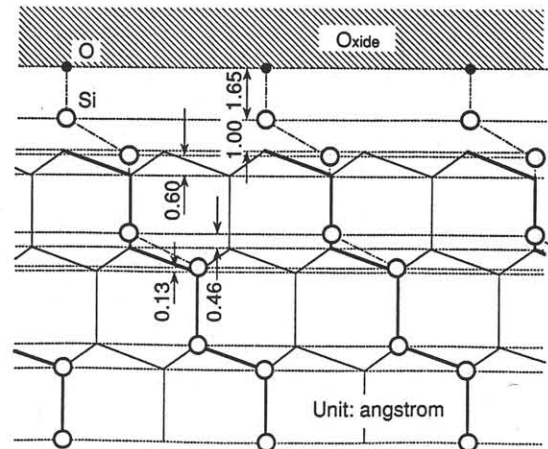


Fig. 5. Model of the interface structure of the native oxide system.

investigating submicron MOS technology.

4. Conclusion

We used MEIS to investigate the atomic structure of the thin $\text{SiO}_2/\text{Si}(111)$ interface.

The Si crystal structure of a thin thermal oxide system is different from that of a native oxide system. From just under the oxide to more than 10 nm deep in the thermal oxide system, the Si atoms are displaced from their ideal lattice positions. A native oxide system, on the other hand, has a relatively simple structure: the top two bilayers of the Si crystal are displaced upward toward the oxide, and there is normal bulk crystal structure underneath.

Structural analysis of the thermal oxide system is being carried out by computer simulation.

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