MRS 1999 Fall Meeting, Boston, Massachusetts, November 29–December 03, 1999

Symposium T: Structure and Electronic Properties of Ultrathin Dielectric Films on Silicon and Related Structures.

ATOMIC AND ELECTRONIC STRUCTURE OF SEMICONDUCTOR/OXIDE INTERFACES

Gerd Duscher,[1] Ryszard Buczko, [1] Stephen J. Pennycook, [2] and Sokrates T. Pantelides[1]

[1]Vanderbilt University, Department of Physics, Astronomy, Nashville, TN;
[2]Oak Ridge National Laboratory, Solid State Division, Oak Ridge, TN.

We use the combination of atom column resolved *Z*-contrast imaging and electron energy-loss spectroscopy (EELS) to study a variety of interfaces between silicon dioxide and semiconductors. A comparison to theoretical calculations (R. Buczko et al.: this symposium) allows one to determine the oxide structures present at the (100) Si/SiO_2 interface. Both silicon substrates with (111) and (100) surface orientation and 4H-SiC substrates were thermally oxidized in dry or wet ambients.

To determine the structure of the crystalline phase of this interface, we use *Z*-contrast imaging in a 300 kV dedicated STEM (VG HB603 U) with a point resolution (FWHM of beam diameter) better than 0.13 nm. With this atom column resolved *Z*-contrast imaging, we determined directly the atomic structure of the substrate at the interface. All the samples had an interface roughness of one atomic layer. This is surprisingly smooth for the SiC/SiO interface, although, at this interface, large accumulated steps due to the misscut are present. The images showed no evidence for crystalline oxide.

The same samples were also studied with EELS at a 100 kV dedicated STEM (VG HB501 UX) with an optimum beam diameter (FWHM) of 0.22 nm. EELS is not only used to study the chemical composition but the electron-loss near edge structure (ELNES) of the ionization edge is (in a first approximation) the local momentum projected density of states of the conduction bands. An analysis of the ELNES of the Si--$L_{2,3}$ and O--K revealed the presence of silicon rich oxide, the basic structure most likely in the form of quartz or cristobalite at the (100) Si--interface. This does not coincide with the equilibrium structure calculated by density functional theory, indicating that there is still room for improvement of this important interface.

*This research was sponsored by the Division of Materials Sciences, U. S. Department of Energy under contract No. DE-AC05-96OR22464 with Lockheed Martin Energy Research Corp.