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Atomic Resolution Z-contrast Imaging and EELS: Application for Ge/SiO_2 Interface

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The technological goal of today's semiconductor industry is the integration of various crystalline and amorphous materials into high-speed silicon integrated circuits. Strained Si on binary SiGe alloys is very attractive for novel band-gap engineered semiconductor devices with significantly improved performances compared to pure silicon. A critical step for the device fabrication is to grow a high-quality dielectric. In the present paper we study a model structure Si/Ge/SiO_2 to understand the processes under the oxidation of strained Si and SiGe.

The Ge film on Si substrate was obtained by Ge ion implantation and successive oxidation. Cross-section [110] samples were prepared by standard mechanical polishing and ion milling. The Si/Ge and Ge/SiO_2 interfaces were studied with a combination of atomic-resolution Z-contrast imaging and electron energy loss spectroscopy (EELS). We used a VG HB603 U dedicated STEM (300 keV, probe diameter less then 0.13 nm) to resolve individual atomic columns in Si or Ge in [110] direction, and the dedicated STEM VG HB501 UX (100 kV) for atomic column resolved EELS [1]. Both STEMs are equipped with aberration correctors.

The analysis of Z-contrast images of Si/Ge/SiO_2 stricture and intensity profiles (fig.1) showed a change of composition of the two atomic layers next to the Ge/SiO_2 interface. EELS data revealed the presence of Si at these layers (fig.2). However, we found that the Si-$L_{2,3}$ ionization edge from the second atomic layer in the crystalline part of the interface has a specific shape. In comparison with a bulk Si, this edge is shifted more than 1 eV towards higher energies and has a different shape (fig. 2, spectrum 3). Also it does not resemble the ionization edge from bulk SiO_2 (fig. 2, spectrum 1). Penetration of oxygen into last two layers is indicated by the O-K ionization edge at the Ge/SiO_2 interface (fig. 3). However, going from bulk SiO_2 towards Ge film, no significant change in the shape and position of O-K ionization edge was detected (compare spectra 1 thru 3). The sub-oxide signature of the O-K edge was not observed.

To model a possible structure of the Ge/SiO_2 interface, we used *ab initio* calculations based on the density functional theory. Calculations showed that from the energy point of view, Ge atoms "prefer" to be far away from the oxide. It is consistent with a number of studies [2, 3] of strained Si, where the rejection of Ge from the oxide layer was observed. Also, it was found that two atomic layers next to SiO_2 are energetically preferred for Si. Combining these results with the experimental data, one can propose the following model. The first atomic layer on the crystalline side of the Ge/SiO_2 interface consists mostly of Si atoms, while the second layer is a mixture of Si and Ge. It is this silicon in the second layer, which gives the specific signature of the Si-$L_{2,3}$ ionization edge. Thus we essentially have an atomic layer of strained silicon. Oxygen (due to the stress in Ge) can penetrate into the first two layers, thus forming stochiometric SiO_2 within the silicon in the first two layers. This model would be consistent with atomically sharp Ge/SiO_2 interface.

To summarize, a combination of Z-contrast imaging, EELS and density functional theory is an excellent tool for semiconductor materials characterization. It allowed us to analyze the structure of the Si/Ge and Ge/SiO_2 interfaces and to detect a compositional change even in one atomic layer. Obtained results can be explained by the proposed model of Si ordering at the Ge/SiO_2 interface.

References

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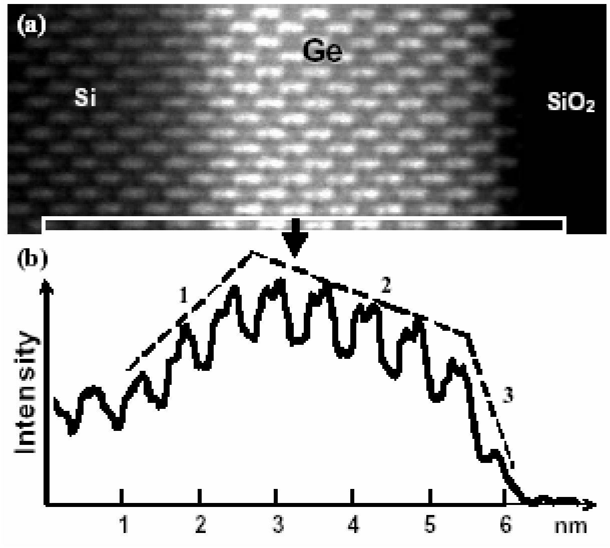

Figure 1. a) Z-contrast image of Si substrate with Ge film covered by SiO_2; b) signal intensity profile across the interface.

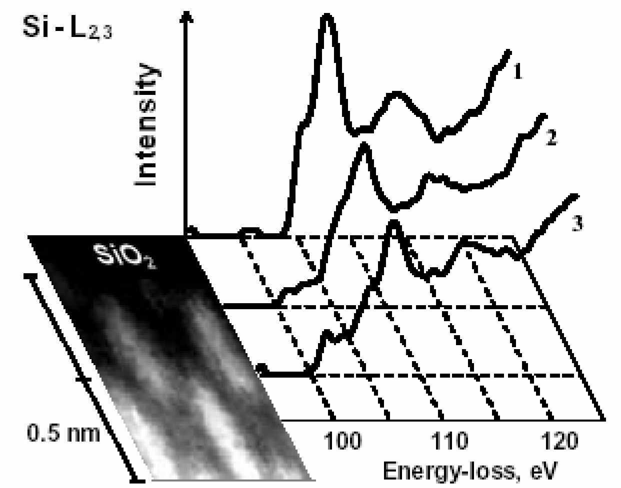

Figure 2. Line-scan EELS of Si-$L_{2,3}$ ionization edge across Ge/SiO_2 interface.

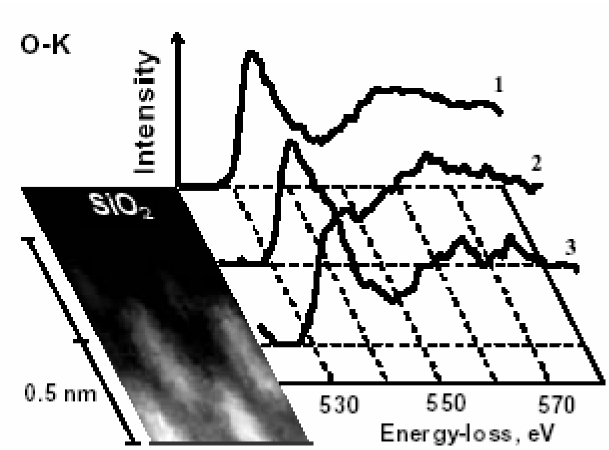

Figure 3. Line-scan EELS of O-K ionization edge across Ge/SiO_2 interface.