DOI: 10.1002/zaac.200670003

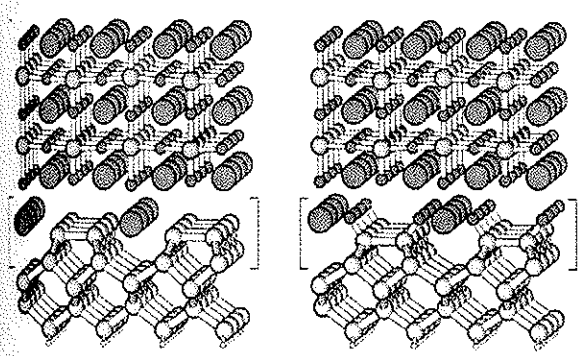
Molecular design of interfaces based on density-functional simulations

Peter E. Blöchl*, C. J. Först, C. R. Ashman, K. Schwarz, A. Reyes Huamantinco

Institute for Theoretical Physics, Clausthal University of Technology, Leibnizstr. 10, D-38678 Clausthal-Zellerfeld

Keywords: Density-functional theory; interfaces; high-K oxides

The ongoing miniaturization of semiconductor devices requires the replacement of the conventional SiO_2-based gate oxides by so-called high-K oxides, in order to avoid quantum mechanical leakage currents through an ultra-thin gate oxide. In the near future, this will require forming interfaces with atomic control and a rational design of the chemical and electrical properties. We discuss the route towards formation of epitaxial high-K oxides with silicon using state-of-the-art electronic-structure calculations and *ab initio* molecular-dynamics simulations.



The goal of this project is to provide insight into the growth processes for molecular beam epitaxy (MBE). In particular, we select the growth of $SrTiO_3$ on silicon, the first demonstrated oxide grown epitaxially on silicon.

The first step is the deposition of the metal atom on silicon. The interaction of the metal ions with the surface reconstruction of the silicon surface exhibits an interesting phase diagram as function of metal coverage. The calculated sequence of phases is relevant for guiding the experimental growth process. The comparison between calculated and measured phase diagrams provides evidence that a solid-state reaction, previously considered vital for forming epitaxial interfaces, is not present. The calculations lead naturally to a new model for the interface structure.

Ab initio molecular-dynamics simulations provide insight into the formation of the oxide on the Sr covered Si surface. It is shown how the interfacial layers provide a covalent template for the semiconductor and an ionic template for the semiconductor.

The interface, being in chemical contact with the oxide, is influenced by the diffusion of oxygen ions to the interface. We investigated how the interface is affected by the addition of oxygen and which interfaces are thermodynamically stable depending on the oxygen partial pressure.

We could show furthermore that the band offsets of valence and conduction bands depend strongly on the oxygen content of the interface. The conduction band offset, called the injection barrier, is a critical device parameter, which tends to be too low for most high-K oxides on silicon. While injection barriers in the range of 1 eV are required, $SrTiO_3$ exhibits a negligible small injection barrier in the range of few tenths of percent. We could show that this finding depends on the oxygen content and that the interfaces can be engineered in such a way that satisfactory injection barriers are obtained.

New developments in semiconductor technology aim at introducing new semiconductors into silicon technology. This requires growth of high-mobility semiconductors such as Ge onto buffer oxides such as $SrHfO_3$. Semiconductor growth on oxides suffers from clustering on the surface. This, however, prohibits the desired layer-by-layer growth mode. On the basis of first-principles calculations it will be shown how the surface can be engineered using surfactants to allow for epitaxial growth of semiconductors on $SrHfO_3$.

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