

Ab initio calculation of reflectance anisotropy spectroscopy of SiC(001) (3×2) surface

Wenchang Lu¹, W. G. Schmidt², E. L. Briggs¹, and J. Bernholc¹

¹*Department of Physics, North Carolina State University, Raleigh, NC 27695-8202*

²*Institut für Festkörperteorie und Theoretische Optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany*

The reflectance anisotropy spectroscopy (RAS) of β -SiC(001) (3×2) surface is calculated within density functional theory in the local density approximation (LDA) using real space multigrid method. A scissor operation is used to correct the underestimate of the band gap in LDA. The results for a two-adlayer asymmetric dimer model (TAADM) are in good agreement with experimental measurements, while the results for other three models (single dimer row, double dimer row and alternate dimer row) do not agree with experiment. The peak located at about 3.5 eV is due to the transition between the occupied dangling bond surface state and bulk-like conduction band, and the peak located at about 5.0 eV is due to the transition between the unoccupied dangling bond surface state and the bulk-like valence band. The transition between occupied and unoccupied surface states is responsible for another peak near 2.0 eV, which is not clearly observed in experiment. Our calculations show that surface states contribute directly to the RAS features of this surface. In addition, it is confirmed that the TAADM is the best model for the (3×2) reconstruction.