Interface induced electronic properties of epitaxial Ag/Si(111) heterojunctions

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Work functions and Schottky barrier heights (SBH) in metal/semiconductor contacts are strongly affected by interface dipole. Density functional calculations within LDA tend to underestimate p-type SBH [1]. We have investigated Ag/Si(111) coincidence site epitaxial system, in order to establish the interplay between the structural and electronic properties at the interface. While the Ag overlayer affects the reconstruction of the Si(111) surface, we find that the geometrical relaxation of the Ag atoms is influenced by the subsurface Si-layer and the concomitant lattice mismatch [2]. The electronic density of states show some oscillations near the Fermi energy, which have been compared with the scanning tunneling spectroscopic (STS) experimental data [2,3]. The signature of metal-induced gap states (MIGS) for this metal–semiconductor heterojunction has been established from the evolution of localized gap states in the layer projected density of states. Our DFT estimates for work function values of the Ag overlayers as well as the p-type SBH of the rectifying Ag/Si contact will be discussed in the light of our current understanding.

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