Modeling STM contrasts of buried interfaces

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Recently, there has been a lot of activity in applying surface microscopy methods to buried interfaces, which are made by growing thin insulating oxide films on top of metallic substrates. Several studies of buried interfaces suggested that it is possible to probe the interface electronic structure via a low-bias scanning tunneling microscopy (STM). However, in many cases the interpretation of the observed STM images is ambiguous. We propose a theoretical method of low-bias STM simulation based on first-principles calculations that allows one to unambiguously interpret the formation of STM images. The method is based on construction of an *ab initio* tight-binding representation of the states near the Fermi level of the system [1]. We apply our method to a prototypical buried interface system: an ultrathin film of rock-salt MgO on top of an Ag substrate. We show that the formation of the STM contrast in this system is dominated by the surface atoms. We show that the low-bias contrast is formed by the states at the Fermi level that originate in the substrate and propagate evanescently through the atomic orbitals of MgO.

[1] A. Malashevich, E. I. Altman, and S. Ismail-Beigi, Phys. Rev. B **90**, 165426 (2014).