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Thin oxide films: analysis of finite-size effects C. FREYSOLDT, P. RINKE, M. SCHEFFLER, Fritz-Haber-Institut, Berlin, Germany — Oxide surfaces have attracted considerable interest over the last years. In order to employ surface science tools, oxides are often grown epitaxially on metals. Recent findings for SiO_2 on Mo(112) indicate that well-ordered films are only 2-3 atomic layers thick – less than previously thought[1,2]. But is the surface of the films characteristic for the surface of a bulk oxide? Not only the structure may differ from any known bulk structure, but also the metal might alter the electronic structure. Also, sizeable quantum effects are expected at these dimensions. We present DFT simulations for oxide films of various thicknesses for SiO_2, Al_2O_3, and HfO_2. In order to separate the thickness from the substrate dependence, free-standing films are considered. We find that the electronic structure at the DFT level becomes bulk-like for very few atomic layers. The case of silica is discussed in detail. The film structure on Mo(112) corresponds to the most stable quartz(0001) surface. The electronic structure is essentially bulk-like and independent of the film thickness. The presence of the substrate does not alter these findings. For the electronic response of the thin film, however, the quasiparticle picture predicts a thickness-dependent band gap due to the dielectric discontinuity at the interface. Likewise, the chemistry and stability of defects is expected to be influenced by the substrate.

[1]L. Giordano *et al.*, Surf. Sci. 584, 225 (2005).
[2]J. Weissenrieder *et al.*, Phys. Rev.Lett. 95, 076103 (2005).

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