Structure of MgO nano-islands on metallic substrates: A semi-empirical, order *N*, Hartree-Fock simulation

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In the last decade, there have been intense efforts to synthesize ultra-thin oxide layers deposited on metal substrates. It has been recognized that, in most cases, their properties largely differ from their bulk analogues, and may be tuned as a function of orientation, thickness and support characteristics. In addition, lateral confinement gives additional degrees of freedom for engineering artificial objects. However, at small sizes, nano-objects are strongly influenced by the interaction with the substrate, both electronically and structurally. This raises questions related to epitaxial growth, formation of Moiré patterns, presence of interfacial dislocations, and elastic relaxation at the interfaces.

In order to decipher the microscopic mechanisms involved, atomistic numerical simulations are of great help. They can complement other approaches based on linear elasticity or theoretical models such as the Frenkel-Kontorova model. However, atomistic simulations of nano-oxides are presently subject to either sever size limitations if first principles methods are used, or suffer from a limited or absent account for the electronic degrees of freedom if classical methods are chosen (extended Born models, chemical potential equalization, etc). We have developed a semi-empirical Hartree-Fock simulation code, which scales quasi-linearly with the system size. It correctly treats the self consistent relationship between the charge distribution and the electrostatic potential acting on the electrons. The adjustable parameters are fitted as to reproduce experimental or first principles results on several periodic systems and on a variety of small clusters. In order to achieve order *N* scaling, a “divide and conquer” strategy is adopted.

We will present the basis of the method, and discuss the epitaxial properties of metal-supported MgO square islands. We will discuss commensurability locking, interface dislocations, island magicity and local electronic properties. We will also show how these properties evolve as a function of the strength of interaction with the substrate and the lattice mismatch, thus producing a “phase diagram” in which size effects will be discussed. Finally, we will make a link with recent experimental results of MgO clusters or layers deposited on Ag(100) and Mo(100).

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