Interface-stabilized exotic phases of metal-on-oxide nanodots

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We discuss a predictive computational methodology which allows one to study the size-dependent epitaxial relationships of metal nanodots supported on (oxide) surfaces. This methodology is first applied to systems with a good epitaxial match, such as Pd clusters on MgO(100), finding results in excellent agreement with experiment [1]. In the presence of a larger lattice mismatch, the possibility of creating unusual metal-on-oxide phases is suggested. In particular, we derive [2] building principles for the formation of "exotic" hcp epitaxies on square-symmetry oxide surfaces, delimiting the values of lattice mismatch, surface and adhesion energy for which hcp phases are expected to be favored even for metals that are not hcp in the bulk. These predictions are supported by available experimental data on Ni/MgO(100) nanodots. Moreover, we are able to rationalize the size-dependent transition from hcp to fcc motifs and to generalize these results to a whole class of metal/oxide systems of great potential interest, such as Pd and Pt on CaO, Ni and Co on MgO. This is the first time that a morphological crossover is quantitatively predicted, a general class of novel nanoparticle phases proposed, and the atomic details of the particle structure fully unveiled for metal-on-oxide particles. Such details in turn suggest that these materials should possess peculiar properties: in particular, the facets exposed by the nanodots reveal adsorption sites with unusual geometry of possible effect on their catalytic properties, while the destabilization of stacking faults and fine details of structural deformations observed for these particles are expected to influence their magnetic behavior.

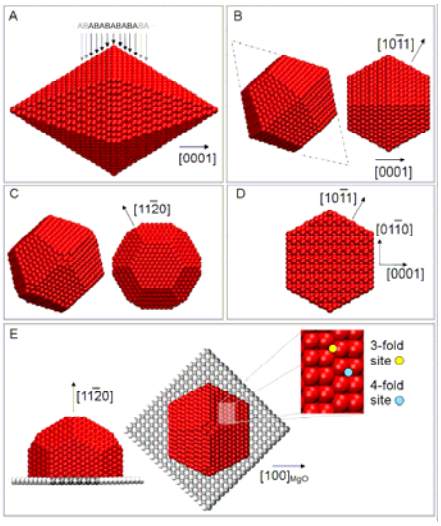

Figure 1: Morphology of the hcp motifs.

[1] G. Barcaro, A. Fortunelli, G. Rossi, F. Nita, R. Ferrando, *Epitaxy, Truncations, and Overhangs in Pd Nanoclusters Adsorbed on MgO(001)*, Phys. Rev. Lett. 98, 156191 (2007)

[2] R. Ferrando, G. Rossi, F. Nita, G. Barcaro, A. Fortunelli *Interface-stabilized exotic phases of metal-on-oxide nanodots* (submitted)