


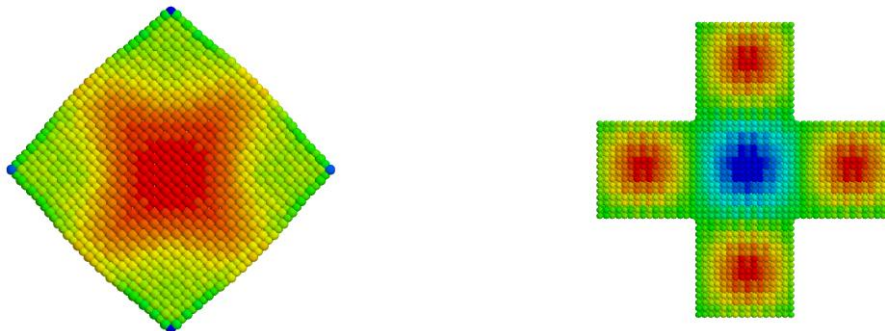
Internship proposal 2011-2012

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Simulation of supported oxide nano-objects

Modern technologies enable fabrication of artificial objects of original and largely unexplored properties. One of major challenges is to master the adjustment of various properties of such objects (shape, structure, stoichiometry, reactivity, etc.) by a simple control of the fabrication environment (temperature, constraints imposed by the substrate, partial pressures of different gases in the fabrication chamber, pH, etc.). The understanding of the driving microscopic mechanisms stimulates a strong demand of realistic numerical simulations.

With a direct relation to experiments in progress in our group, we propose a computational study on the shape and atomic structure of small oxide objects, such as MgO and ZnO, deposited on a metal substrate. We are going to focus on the effect of elastic constrains due to lattice mismatch between oxide nano-object and the support: structural distortions (e.g. interface misfit dislocations which produce a Moiré effect, to be seen in the map of local pressure on the left) or changes of shape (e.g. stabilization of cross-like shapes, pressure map on the right).



Simulation of the substrate-induced constrain as a function of object size will aim an identification of experimentally accessible parameters which may enable practical fabrication of nano-objects of desired size, shape, and structure. The study will rely on an original computational approach developed in our group.

Applicant skills :

Master in material science

Granted internship : yes (~400 €/month)

C'nano IdF laboratory (France only) : yes

Possibility for a thesis : yes (type of grant : scholarship by French ministry)