MASTER DE PHYSIQUE ET APPLICATIONS - 2ème année
Spécialité Sciences des Matériaux et Nano-objets
International Nanomat Master Program

Internship proposal 2009-2010

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Nano-oxide dielectrics: « material design » with a computer

Recent years have seen substantial advances in high performance logic and memory devices in which increasingly complex oxides are being incorporated, usually as thin films, due to their diverse characteristics (dielectrics, ferroelectrics, ferromagnets, metals, transparent conductors, tunnel barriers, piezoelectrics, sensors, etc.). While oxide dielectrics are currently used in a large variety of applications with specific requirements for dielectric constant (k), thickness, leakage, band-gap, band-offset, breakdown voltage, and defect density, the industry is constantly very actively searching for new, better performing ones.

The goal of this theoretical internship/thesis is to identify the microscopic mechanisms responsible for specific electronic and dielectric properties (band alignment, interfacial charge transfer, polarization, etc) of metal-oxide interfaces involving novel interface orientations, symmetries, and stacking sequences in the oxide - the parameters that can be tailored during device fabrication by using either specific substrates or oxide films with specific structures and stoichiometries.

The proposed methodology relies on first principles DFT methods for the exploration of the structural phase diagram of ultra-thin oxide films and for the theoretical characterization of electronic and dielectric characteristics on the most accurate level. Indeed, as film thickness decreases, unexpected new structures can be stabilized, largely different from the bulk ones, and strongly dependent upon the fabrication conditions. Properties of such nano-oxides are entirely to be discovered and explored, with the goal to give guide-lines for engineering their dielectric characteristics.

Techniques in use :
"Ab initio" Numerical simulation

Applicant skills :
Basic theoretical description of the electronic structure of solids.

Granted internship : yes (280 €/month)
C'nano IdF laboratory (France only) : yes
Possibility for a thesis : yes (type of grant : scholarship by French ministry)