Growth of materials through vapor-like deposition process in the context of Microelectronic: understand the atomic scale to design the matter

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Résumé

Mastering interfacial layers is the current challenge for nanotechnologies when materials are directly integrated into devices. Interfacial layers are inevitably formed during technological fabrication notably during vapor-like deposition processes. As integrated layers now reach a nanometer thickness, atomistic composition and structure of the interfacial layers become preponderant and play a determining role on the macroscopic properties of designed materials.
To push forward the nanoscale–controlled fabrication of integrated materials, predictive atomic scale modeling of the deposition process can help, by providing a fundamental description on how they are achieved. It appears as a challenging task, since dynamics involved in matter organization span a large range of time and size scales.

To overcome this issue, multi-levels modelling approach is strategic [1-5]. Here, Density Functional Theory-based (DFT) calculations [6] or DFT/ART coupling [7] (Activation Relaxation Technique) are first used to identify and characterize, kinetically and thermodynamically, atomic scale events, and then are implemented as input parameters to parameterize a kinetic Monte Carlo (KMC) model. KMC methodology is well identified for the simulation of the growth of materials with an atomistic insight. It allows to carry out simulations by varying deposition parameters and predict influence of these parameters on interfacial layer formation.

In this presentation, I will describe how this strategy is developed on deposition of CuO on Al(111) and on silicon oxidation. As activation barriers are the key parameters for a good calibration of kMC methodology, a focus will be given on atomistic investigation: the dynamic features relative to atomic diffusion (notably the activation barriers) during the interface growth are highly dependent on local physical properties.

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