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An atomistic insight into interface formation in directly integrated materials: a modeling study of CuO deposition on Al(111) through DFT-kMC approach

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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. In our approach, we propose a model based on a kinetic Monte Carlo (KMC) methodology to simulate the growth of materials as a function of the deposition parameters with the overall goal of getting clues, depicting and predicting the realistic interfacial formation [1,2]. Here, Density Functional Theory-based (DFT) calculations are first used to identify and characterize, kinetically and thermodynamically, atomic scale events, that are then used as input parameters to parameterize a KMC model (Figure 1).

This methodology offers the possibility to access to the exact structure of the material as a function of the manufacturing process and thus to access to the detailed composition, that depends on the conditions in which it was synthesized. We expect to propose microscopic elements that could guide the technologist to improve processing and improve the properties of the operating material.

This methodology will be illustrated on CuO deposition onto Al(111) substrate, where CuO/Al thermites are used as energetic materials deposited as nanometer-thick multilayered materials through sputtering process [3] (Figure 2). They are directly integrated into devices as micro-sources of energy. The interesting point of these materials is the intimacy of Al and CuO components, that can be customized to tailor macroscopic properties. Actually, it has been proven that interfacial layers impact final performances of achieved materials, such as stability, reactivity and energy release. In this field, master of interfaces during their fabrication is a major issue since it offers the new opportunity to increase and tune their final performances.

Presented results will include CuO chemistry on the Al surface [4,5], and the early stages of PVD deposition will be examined up to the complete passivation of the Al surface (Figure 3).

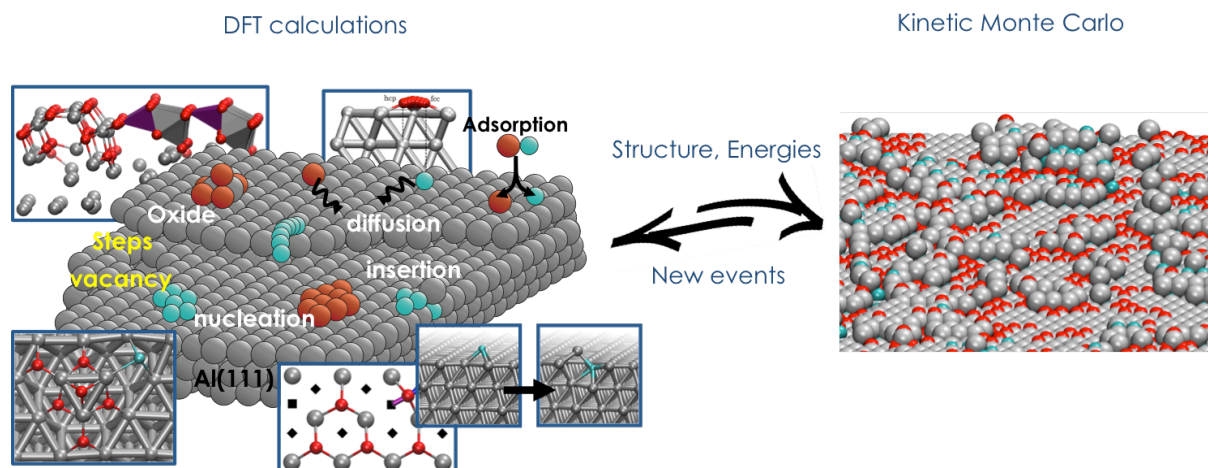


Figure 1. DFT-KMC approach

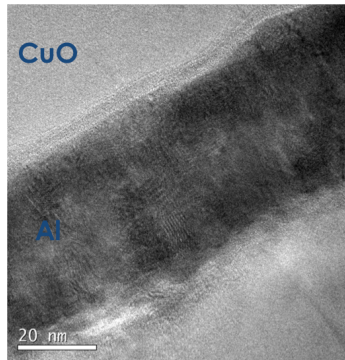


Figure 2. Multilayered CuO/Al energetic materials [3]

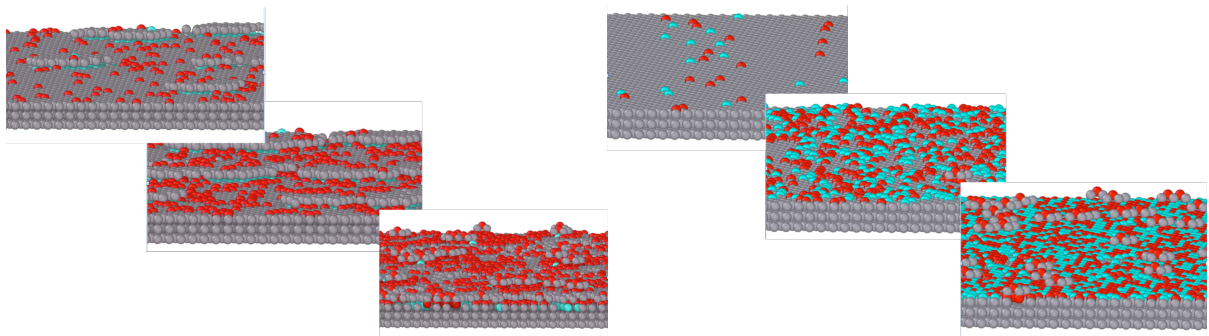


Figure 3. kMC simulations of CuO on Al(111) at 30°C (left) at -140°C (right).

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