

An Atomic Scale Insight into Interface Layers Formation in Al/CuO Nanolaminated Thin Films: a Kinetic Monte Carlo Simulation of Deposition Process

M. Guiltat^{1,2}, A. Estève^{1,3}, C. Rossi^{1,3}, M. Djafari-Rouhani^{1,2}, Y.J. Chabal⁴ and A. Hémerlyck^{1,3}

¹CNRS, LAAS, 7 avenue du Colonel Roche, F-31400 Toulouse, France

²Univ de Toulouse, UPS, LAAS, F-31400 Toulouse, France

³Univ de Toulouse, LAAS, F-31400 Toulouse, France

⁴Department of Materials Science and Engineering, University of Texas at Dallas, Richardson, Texas 75080, USA

Nanolaminated materials made of nanometer-thick layers are nowadays facing the technological challenge of mastering interfacial layers, inevitably formed during technological fabrication processes. At these dimensions, interfacial layers become preponderant and play a determining role on the macroscopic properties of designed materials.

In nanolaminated energetic materials, more precisely multilayered Al/CuO nanothermites, in which intimacy of Al and CuO components must be maximized, it has been proven that interfacial layers, still unknown in composition and not well controlled during processing, 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 performances as for example in the perspective of their integration into MEMS technologies.

Actually, multilayered nanothermites suffer from a lack of knowledge of the structure and composition of both the deposited layers and interfaces, with an atomic scale precision, in relation with the deposition process parameters (temperature, partial pressures ...).

To push forward their nanoscale-controlled fabrication, predictive atomic scale modeling of the deposition process can help, by providing a fundamental description on how they are achieved. Simulations appear here as a powerful tool for the characterization of phenomena occurring at the nanoscale as a deep dive into the matter, to guide the technologists toward the development of advanced nanostructured materials. In our approach, we propose a model based on a kinetic Monte Carlo (KMC) method to simulate multilayered Al/CuO materials deposition, as PVD process, in order to get clues, depict and predict a realistic interfacial formation. Here, Density Functional Theory-based (DFT) calculations are used to identify and characterize, kinetically and thermodynamically, atomic scale events. Then these DFT data are used as input parameters to parametrize a KMC model. Presented results will include CuO chemistry on the Al surface, and the early stages of PVD deposition will be examined up to the complete passivation of the Al surface. 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.