Nanostructured Energetic Materials: Fabrication process and atomic scale modeling

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Nanoenergetic materials and reactive nanolaminates have attracted great interest in the energy generating material community since they are characterized by a high energy density (superior to supercapacitors), are low cost and safe. In recent years, ideas have emerged to integrate them into micro and nanosystems opening the route to nanoenergetics on a chip with applications in civilian as well as military fields: environmentally safe and clean primers and detonators, smart and fast fuses, nanoscale heat sources for biological and chemical neutralization and disease treatment.

At LAAS, our team is already oriented towards the creation of new generations of nanostructured energetic materials and nanolaminates. Al-CuO nanolaminates are magnetron sputter deposited from Al and Cu targets using DC power supplied, on oxidized silicon wafer. Many hundreds of nanometer thick layers can be stacked by alternating oxidizer and fuel. Each reactant layer thickness can be accurately set at +/- 5nm and the layering also places the reactants in intimate contact leading to a reduction of the diffusion distance by a factor of 10-1000 compared to the same material traditionally prepared by powder mixing. During vapor deposition, invariably an intermixing occurs at the Al and CuO interface. These intermixed interfaces play a critical role during the synthesis and the utilization of the material. The formation of interfacial layers is not only poorly understood but uncontrolled at present. An understanding of the formation, role and control of these interfacial layers is among the most important technological issues in highly reactive materials. We have developed atomic scale process simulation based on DFT calculations to depict elementary chemical and also incorporating a novel accelerated Molecular Dynamics scheme (hyperthermal Kinetic Monte Carlo) into conventional Kinetic Monte Carlo to overcome issues associated with exothermic reactions. This will lay the foundation of a TCAD (Technology Computer Aided Design) dedicated to reactive nanolaminates.

A second technological approach, also developed at LAAS, is to direct the assembly of nanoparticles of Al and CuO into a micron size Al-CuO composite particle thanks to DNA strands [1]. While the potential of this technology has been recently demonstrated in the liquid phase (AFM), surface integration is still an open issue. Because of the bio-hybrid intrinsic complexity of these systems, a fundamental basic understanding is required. First principles calculation are therefore combined with technology to guide the assembly procedure and choices: surface modification strategy, grafting, solvent issues…

Besides this work, clean room facilities and infrastructures of LAAS, as the activities around the project TRAIN2, will be discussed.

[1] F. Séverac et al., Adv. Func. Mat. 22 (212) 323.