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Impact of the granularity of a high-explosive material on its shock properties

Xavier Bidault and **Nicolas Pineau**
CEA DAM/DIF, France

Recent experimental studies show that granularity has a substantial impact on the detonation behavior of high-explosive materials: under shock loading, a nanostructured one leads to smaller nanodiamonds than a microstructured one [1]. Moreover, simulations show that a porous energetic material undergoes an extra temperature rise related to the size of the pore/defect [2, 3]. Two aspects of this granularity, the surface energy and the porosity, are explored to investigate these different behaviors. From a model energetic material, the surface energy of nanoparticles with a radius from 2 nm up to 60 nm has been determined by means of Molecular Dynamics simulations using ReaxFF-lg potential [4]. Then, using the Rankine- Hugoniot relations and the equation of states of the corresponding bulk material [5], the contribution of this excess energy to the heating of the shock-compressed, nanostructured and porous material is determined, and compared to the compaction work needed to collapse its porosity. This allows evaluating the balance of these two aspects of granularity to the extra temperature rise under shock loading.

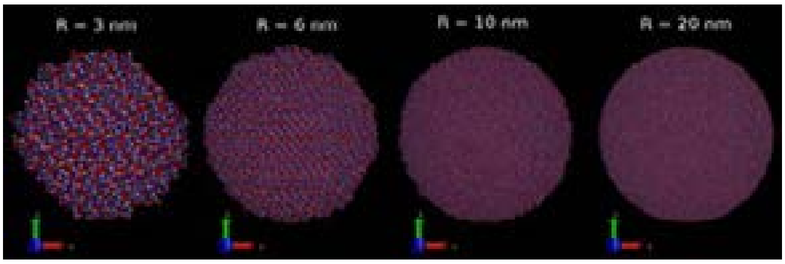

Figure1: Nanoparticles of the model energetic material

Biography

Xavier Bidault has his expertise in modeling and analysis of nanostructured materials by Molecular Dynamics. In order to study nanostructured optical fibers, the simple adaptive model that he developed during his Physics PhD allowed the simulations to reproduce for the first time the separation of phases of complex compositions in silica-based glasses, as experimentally observed. He now enlarges his skills to organic materials to understand how the granularity (surface energy and porosity) of a nanostructured energetic material impacts its reactivity under shock, with a focus on nanodiamond formation.

xavier.bidault@cea.fr

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