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Formation of carbon-based nanostructures from carbon suboxide decomposition at high pressure and temperature – A ReaxFF study

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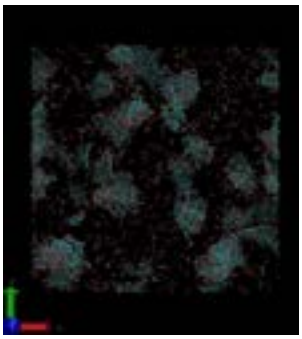
In high-pressure and -temperature conditions of detonation, carbon-rich explosives produce carbon-based nanostructures like Nano diamonds. The formation process from these organic compounds is still not clear and the published Molecular Dynamics studies are either limited to carbon condensation with no chemistry, which is quite basic, or by computer resources when modeling systems with full "carbon-hydrogen-oxygen-nitrogen" chemistry, preventing long-time simulations. As the formed nanostructures are mainly composed of carbon and oxygen (with low amounts of hydrogen and nitrogen), An intermediate system between non-reactive and full-chemistry ones can be represented by carbon sub oxide (C_3O_2), in mixture with Argon. When modeled with a reactive force field (ReaxFF-lg, this system catches experimental results of low-pressure detonation (~10 bar) and allows extrapolations in the high-pressure domain of solid-state high-explosive detonations (up to 60 GPa). In these extreme conditions, it appears that the formation process of carbon-based nanostructures is deeply modified and the results obtained from this reactive carbon-oxygen system give new insights on the formation of Nano diamonds.



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 Nano diamond formation.

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