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Atomistic simulations for granular explosives under shock compression[1] NICOLAS PINEAU, XAVIER BIDAULT, CEA/DAM/DIF — Solid explosives are composite materials made of molecular crystal grains binded by a polymer matrix. Although most of their detonation properties are related to the explosive molecule itself, the granular structure can give a non-negligible contribution due the stacking porosity, the granular surface energy, or the properties of the binder: for instance detonation nanodiamonds synthesized from carbon-rich explosives display granularity-dependent size-distributions. We present a series of numerical studies based on molecular dynamics simulations which aim at improving our understanding of the impact of granularity on the shock/detonation behavior of these solid explosives. We show that their shock-induced properties depend mostly on the initial porosity amount and structuration. The local perturbation of the shock temperature and pressure are likely to modify the chemical decomposition process, suggesting a potential impact on the detonation products.

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