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Surface energy of explosive nanoparticles NICOLAS PINEAU, XAVIER BIDAULT, LAURENT SOULARD, CEA DAM DIF — Recent experimental studies show that nanostructuration has a substantial impact on the detonation of high explosives: a nanostructured one leads to smaller nanodiamonds than a microstructured one (Pichot et al, Sc. Rep, 3 (2013), 2159). Whether it comes from a higher surface energy or from porosity, the origin of these different behaviors must be investigated. The surface energy of TATB nanoparticles with a radius from 2 nm upto 60 nm has been determined by means of ReaxFF-based simulations. Then, using the Rankine-Hugoniot relations and the equation of states of the bulk material, the contribution of this excess energy to the heating of a shock-compressed nanostructured (and porous) material is evaluated and compared to the thermal effect due to its porosity collapse. A maximum temperature increase of 50 K is found for 4-nm nanoparticles, which remains negligible when compared to the few hundred degrees induced by the compaction work.

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