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Molecular dynamic and kinetic study of carbon cluster aggregation in detonation products thermodynamic conditions. GUILLAUME CHEVROT, ARNAUD SOLLIER, NICOLAS PINEAU, CEA/DAM/DIF — The detonation of carbon-rich explosives produces significant amounts of solid carbon residues that interact with the surrounding fluid mixture, modifying the equation of state of the detonation gas. The formation process of the solid carbon phase and its influence on the detonation products has been investigated for a decade through atomistic simulations and kinetic models but some questions remain about the coalescence mechanism and kinetics, in particular on the influence of the variation in thermodynamic properties during the gaseous product release. In this study, we present a combined molecular dynamics and kinetic study of the solid carbon clustering process in thermodynamic conditions relevant for the release of high explosive detonation products. First we use molecular dynamics simulations based on the LCBOPII potential to investigate the coalescence mechanism of nanocarbons under high temperature and pressure: under those conditions coalescence occurs whenever two carbon clusters approach to within the potential dispersion interaction range. Then we implement this statistical observation as well as various physically-based features to a Smoluchowski model to investigate the kinetics of aggregation of carbon, and draw qualitative comparisons with the available experimental observations.

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