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Theoretical study of the porosity and temperature effects on the shock response of graphitic materials EMERIC BOURASSEAU, NICOLAS PINEAU, DAVID HEBERT, LAURENT SOULARD, CEA — The response of graphite, and graphite-like materials, to shock compression have been the subject of numerous experimental studies over a few decades, showing a substantial dependence of the shock properties (Hugoniot curves, transition to diamond, ...) on the initial porosity and granularity of the polycrystalline samples. Theoretical studies of these processes have been enabled only recently, thanks to the development of computationally efficient empirical potentials such as LCBOPII which reproduce accurately the various phases of carbon (graphene, graphite, diamond, liquid carbon) and the few available ab initio data for shock compression of graphite. These studies are restricted to monocrystalline samples which, in the case of graphite, represent a serious approximation to the actual experimental set-ups and may explain the large over-estimation of the graphite/diamond transition pressure ($\sim$ 60 GPa vs. 15-25 GPa). In this paper we present a theoretical study on the shock compression of porous graphite by means of Molecular Dynamics and Monte Carlo simulations using the LCBOPII potential. The results are compared to the available experimental data and the role of porosity and temperature on the shock properties and graphite/diamond transition is discussed.

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