Atomistic simulations of shock loading on single and nanocrystalline SiC ceramics

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Molecular-dynamics simulations of plane shock loading in single and nanocrystalline SiC are performed to investigate the generation and interplay of shock-induced compaction, structural phase transformation and plastic deformation. The shock profile of single crystalline SiC is calculated for a wide range of particle velocity from 0.1 km/s to 6 km/s and along the [001], [011], and [111] crystallographic directions. The calculated Hugoniot curves agree well with the experimental one. Shocks on different crystallographic directions indicate the generation of elastic shock wave for shock loading below 2 km/s. For intermediate particle velocity, between 2 km/s and 5 km/s the generated shock wave splits into an elastic precursor and a zinc blend-to-rocksalt structural transformation wave. That is induced by the increase in shock pressure to over 90 GPa and results in increase of density to ~4 g/cm^3. A twinning based plastic wave is generated ahead of the transformation wave for shocks on the [001] and [111] directions. For particle velocity greater than ~4-5 km/s a single overdriven transformation wave is generated. We further examined the effects of grain boundaries and grain sizes on the generated shock Hugonot curves and compared with the results of single crystalline SiC. In particular we discuss the nanocrystalline effect in the generation of plastic deformation. These simulation results provide an atomistic view of the dynamic effects of shock impact on single crystal and nanocrystalline high-strength ceramics.

Keywords: shock, Hugoniot curve, plastic deformation, structural transformation, SiC, ceramics