Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

Atomistic modeling of the dynamic behavior of single and nanocrystalline SiC under plane shock loading PAULO BRANICIO, JINGYUN ZHANG, Institute of High Performance Computing, Agency for Science, Technology and Research, AIICHIRO NAKANO, RAJIV KALIA, PRIYA VASHISHTA, University of Southern California — The dynamic behavior of SiC in single and nanocrystalline samples is investigated by classical molecular-dynamics simulations of plane shock loading. The generation of elastic shock induced compaction, plastic deformation, and pressure induced structural phase transformation is characterized as a function of impact crystallographic direction ([001], [011], and [111]) and temperature (10 K & 300 K). Shock profiles are calculated in the wide range of particle velocity from 0.1 km/s to 6 km/s. The predicted Hugoniot curves agree well with available experimental data. Results indicate the generation of elastic waves for shocks below 2 km/s. In the intermediate range of velocities 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, which is triggered by the increase in shock pressure to over 90 GPa and results in increase of density to ~ 4 g/cm3. A plastic wave is generated ahead of the transformation wave for shocks on all crystallographic with clear signs of twinning. For particle velocity greater than 4-5 km/s a single overdriven transformation wave is generated. We further examined the effects of grain boundaries in nanocrystalline samples on the generated shock Hugoniot curves. In particular, we discuss the generation of plastic deformation and the absence of shock wave splitting.

Paulo Branicio
Institute of High Performance Computing

Date submitted: 30 Jan 2015 Electronic form version 1.4