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Shock-induced phase transformations in silicon: continuum and x-ray diffraction measurements[1]

STEFAN TURNEAURE, Washington State University

Silicon under static compression undergoes a sequence of structural transformations with increasing pressure [Mujica et al., Rev. Mod. Phys. 75, 863 (2003)]. Previous dynamic compression experiments on silicon using different drivers and various diagnostics have not provided observations of any high-pressure silicon crystal structures but have raised many questions. For example, impact loading of millimeter scale thickness Si(100) samples from 16-22 GPa results in the formation of 3 shock waves transmitted through the material [Turneaure and Gupta, Appl. Phys. Lett. 91, 201913 (2007)]. The first wave compresses the silicon elastically and at the HEL (9 GPa) the stress deviators are large. Inelastic deformation occurs in the second wave, but the mechanisms responsible for relaxation of the stress deviators are not understood. Continuum and x-ray diffraction (XRD) measurements demonstrate that the stress deviators remain nonzero between the HEL and the phase transformation stress [Turneaure and Gupta, J. Appl. Phys. 111, 026101 (2012)]; the role of the stress deviators on the structural changes in silicon is an open question. A large volume collapse occurs in the third (phase transformation) wave with the peak state stress-density being consistent with one of the high-pressure structures observed for statically compressed silicon, but the structure in the peak state could not be determined from earlier experiments. Using multi-frame powder XRD measurements at the Dynamic Compression Sector the crystal structure of polycrystalline and single crystal silicon shock compressed to 26 GPa (and then partially released to 19 GPa) was directly examined [Turneaure and Gupta, Phys. Rev. Lett. 117, 045502 (2016)]. Both polycrystalline and single crystal silicon were found to transform to the simple hexagonal structure under shock compression. An important finding was that shock compression of single crystal silicon resulted in a highly textured simple hexagonal phase. Comparison of diffraction simulations for textured simple hexagonal silicon with the measured diffraction patterns revealed the orientation relations between the ambient cubic diamond and simple hexagonal silicon structures. The experimental approach and analysis procedures are general, and are being used at the Dynamic Compression Sector to examine orientation relations between low and high-pressure structures in other shocked single crystal and textured materials.

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