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Atomistic Calculations of Nanosecond Timescale Kinetics of Shock-Compressed SiO2

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Unraveling the behavior of SiO2 under high dynamic pressures is important for understanding meteor impacts, laser-induced damage of optics, and interpretation of shock compression experiments in a geophysical context. This behavior is made complicated by the presence of several high pressure phases and complex kinetic processes that yield long-lived metastable states. Quantitative understanding of the kinetics is nearly as important as the thermodynamics for this material. Here we make the first atomistic calculations of kinetic processes in SiO2 shocked to pressures near the stishovite and melt boundary. We perform atomistic calculations with up to 1 million atoms for timescales of 10 nanoseconds to elucidate the nucleation and growth and subsequent grain size evolution of the stishovite phase. These calculations are enabled by the multi-scale shock technique (MSST) implemented in LAMMPS. We further study the role of the quantum nature of the nuclei at 1 million atom scales using a fast semiclassical variation of MSST called QBMSST.