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Nanosecond Timescale Homogeneous Nucleation and Crystal Growth in Shock-Compressed SiO_2 YUAN SHEN, SHAI BARAK, TINGTING QI, EVAN REED, Stanford Univ — Understanding the kinetics of shock compressed SiO2 is of great importance for mitigating optical damage for high intensity lasers and understanding meteoroid impacts. Experimental work has placed some thermodynamic bounds on the formation of high pressure crystal phases, but the kinetics and microscopic mechanisms are yet to be elucidated. The latter are particularly relevant for this material which has long-lived metastable states. Enabled by million atom multiscale shock technique (MSST) molecular dynamics studies of shock compressed fused silica and quartz using variations on the BKS analytical potential, we discover here that crystallization occurs within as little as a few nanoseconds. In surprising contrast to shock induced solid-solid phase transformations in metals, we find that the transition from quartz obeys a diffusion mediated homogeneous nucleation and growth model due to formation of an intermediate disordered phase. We construct a quantitative model of diffusion mediated nucleation and growth kinetics and compare to stishovite grain sizes observed in laser damage events and near the Barringer Crater. We also study the effect of quantum nuclear effects using the quantum bath MSST and find that shock temperatures are shifted up to 500 K from classical values.

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