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Quantum molecular dynamics simulations of beryllium at high pressures[1] MICHAEL DESJARLAIS, MARCUS KNUDSON, Sandia National Laboratories — The phase boundaries and high pressure melt properties of beryllium have been the subject of several recent experimental and theoretical studies. The interest is motivated in part by the use of beryllium as an ablator material in inertial confinement fusion capsule designs. In this work, the high pressure melt curve, Hugoniot crossings, sound speeds, and phase boundaries of beryllium are explored with DFT based quantum molecular dynamics calculations. The entropy differences between the various phases of beryllium are extracted in the vicinity of the melt curve and agree favorably with earlier theoretical work on normal melting. High velocity flyer plate experiments with beryllium targets on Sandia's Z machine have generated high quality data for the Hugoniot, bulk sound speeds, and longitudinal sound speeds. This data provides a tight constraint on the pressure for the onset of shock melting of beryllium and intriguing information on the solid phase prior to melt. The results of the QMD calculations and the experimental results will be compared, and implications for the HCP and BCC phase boundaries of beryllium will be presented.

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