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Multiphase equation of state and strength properties of beryllium from ab initio and quantum molecular dynamics calculations GREGORY ROBERT, ARNAUD SOLLIER, CEA-DIF BP 12 91680 Bruyeres le Chatel — In the framework of density functional theory, static properties and phonons spectra of beryllium have been calculated under high compression (for pressures up to four Mbar) for two solids phases : hexagonal compact (hcp) and body-centred cubic (bcc). The melting curve and some isotherms in the liquid phase are calculated using quantum molecular dynamic. The coupling of these theoretical data to a quasi-harmonic approach (Debye model) for these three phases (two solids and a liquid) allows us to suggest a new theoretical phase diagram as well as a multiphase equation of state in a large range of pressure and temperature. The resulting 300K isotherm and Hugoniot curves as well as the evolution of the shear modulus with both pressure and temperature are in good agreement with available data. The elastic constants calculated under shock loading allow us to fit the coefficients of constitutive laws at very high pressures and high strain rates.

Gregory Robert
CEA-DIF BP 12 91680 Bruyeres le Chatel

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