

Predicted Dehydration of Brucite (Mg(OH)₂) to Periclase (MgO) at High Pressures and Temperatures Using Local Basis Function Energy Representations

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The dehydration reaction of brucite to periclase + water is an ideal system to test the accuracy of energy representations for solids and fluids under elevated pressures and temperatures. Substantial experimental effort has gone into measurements for all three materials. Here, available measurements are reviewed, and new local basis function energy representations are created for the solids. Both harmonic and anharmonic contributions to Helmholtz energy are included during correlation with high pressure and high temperature measurements of volumes, vibrational modes (Raman and infrared), and elastic moduli. Combined with a representation for water and water with NaCl, the phase boundary for brucite dehydration is determined and compared with other predictions and the experimentally determined phase boundary. The currently predicted boundary agrees with experiment to near 4 GPa and 1400 K. At higher pressures the experimental phase boundary remains near 1400 K while the predicted boundary trends to high temperatures; the predicted dehydration temperature is 200 K high at 8 GPa. Such deviations from experiment may be associated with the assumption that pure water is the equilibrium phase. Increasing solubility of MgO in water would reduce water activity and depress the dehydration temperature. Under the assumption that the energy representations and determinations of phase boundaries are all accurate, constraints on MgO solubility under these extreme conditions are possible.