A semi-empirical multiphase equation of state for aluminum

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Energies of face-centered cubic (fcc), hexagonal close-packed (hcp) and body-centered cubic (bcc) aluminum phases were calculated with the all-electron full-potential linear muffin-tin orbital (FP-LMTO) method for relative volumes (V/V_0) in the range from 0.25 to 1.05. Phonon spectra were calculated in the same range within linear response theory and used to determine the contribution of lattice vibrations to the free energy in quasi-harmonic approximation and to construct a phase diagram for aluminum. The melting curve was obtained from the Lindemann criterion. Also, calculations were done to determine the thermodynamic functions of aluminum in the region of its liquid and plasma states in the average-atom model RESEOS. Results of our calculations along with experimental evidence were used to construct a multiphase (fcc, hcp, bcc, liquid + evaporation) equation of state for aluminum. The fcc, hcp and bcc equilibrium lines, the melting and evaporation curves, and critical point parameters were obtained from calculations. The resulted semi-empirical equation of state is shown to agree well with experimental and calculated data in a wide range of temperatures and pressures.