

Physical contradictions and remedies using simple polythermal equations of state

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ABSTRACT

Simple polythermal extensions to two widely used isothermal equations of state, the Murnaghan and the Birch-Murnaghan, can lead to non-physical material behavior without proper parameterization: the thermal expansivity at high pressure can become negative. We show how this arises and propose a remedy using an approximation to the thermal relaxation of the bulk modulus. Using the revised equation of state for thermodynamic equilibrium calculations leads to low-pressure and -temperature behavior indistinguishable from the unmodified equation of state, yet extrapolates to high pressure and temperature without non-physical behavior.

Keywords: Thermodynamics, equation of state properties, phase equilibria, calculation, high-pressure studies, expansivity measurements, negative expansivity