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Application of free volume theory to the model of thermal pressure for NaCl

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Mie-Gruneisen type equation is frequently used for the Temperature-Pressure-Volume equation of state (EoS) for pressure standard materials and minerals in the Earth's interior. Mie-Gruneisen type equation consists of the isothermal compression term and the thermal pressure term. In the thermal pressure term, Gruneisen parameter (γ) is very important thermodynamic parameter. It is known that γ relates to the property of isothermal compression as Slater's equation [1]. From the studies of molecular dynamics and potential theory, Barton and Stacey [2] advanced the free volume theory [3], and then derived the equation (called as "modified free volume formula" or "Barton-Stacey formula"), which can calculate practical γ values from the parameters of an isothermal compression curve. It is important that this formula gives theoretically support for volume dependence of γ, and moreover reduces the parameters of total EoS in number.

In this study, we apply Barton-Stacey formula to NaCl-B1 phase. We use the CT-EoS data as experimental reference, and the thermal pressure model, which include effect of intrinsic anharmonicity, as base model [4]. The power law γ at zero temperature in the base model is replaced by Barton-Stacey formula with the parameters of the isothermal EoS at zero temperature [5,6]. The value of f, which is the parameter relating to the randomness of thermal motion of atoms in Barton-Stacey formula, is estimated from using the free volume γ [3]. The present model reproduce successfully values of γ and specific heats without sacrificing accuracy, in spite of reducing one parameter of the EoS.

References

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