Shifts in thermal expansivity with Fe content for solid solutions of MgSiO₃-FeSiO₃ with the perovskite structure

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ABSTRACT

This study presents evidence that for a solid solution of Mg₂₋ₓFeₓSiO₃ perovskite, the shift in volume thermal expansivity, $\alpha$, is small as the index $x$ is changed. According to data obtained theoretically by Hama and Suito (1998), $\alpha$ decreases by 0.3–0.4% as $x$ changes from 1 to 0.9 in a temperature range of 1900 K. Furthermore, the relative shift in $\alpha$ for Fe substitution is similar to that found by recent measurements of MgSiO₃ perovskite (Fe-free perovskite, or simply Pv) found by Mao et al. (1991) and Knittle et al. (1986), as Jeanloz and Hemley (1994) had predicted.

In an attempt to reconcile the data in Figure 1, it could be conjectured that the high $T$ values of $\alpha$ for Fe-Pv arise from the Fe itself (e.g., a considerable shift occurs in $\alpha$ with Fe content). A recent theoretical paper shows such a conjecture to be unfounded. Hama and Suito (1998), solving for thermoelastic constants using the Vinet equation of state, demonstrated that Fe-Pv and Pv yield virtually the same value of $\alpha$ at the $P$ and $T$ conditions of the lower mantle (see their Fig. 11). The data behind Figure 11 of Hama and Suito (1998) are listed in Table 1 here.

Thermodynamically, this study shows that the shift in $\alpha$ going from Pv to Fe-Pv is small by exploiting the properties of a Debye solid. MgSiO₃ perovskite has been proven to be a Debye-like solid by showing that using the Debye theory for Pv produces values of four thermoelastic parameters that agree with those measured or calculated by others (Anderson 1998). Further proof is shown in Table 2, which lists the values of $K'_v$ (isothermal bulk modulus), $K'_s$ (adiabatic bulk modulus), $v_s$ (longitudinal sound velocity), $v_p$ (shear velocity), and $\gamma$ (Grüneisen parameter), all vs. $T$, from both the Anderson (1998) Debye calculation and the Hama and Suito (1998) calculation. This table shows general agreement between the results from the Debye model and those from the theory based on the Vinet equation of state. The calculated volumetric thermal expansion of Fe-Pv $\alpha$ data is in good agreement with those measured for Fe-Pv.

INTRODUCTION

Figure 1 introduces the problem to be discussed here. The measured and calculated volume thermal expansivity, $\alpha$, of MgSiO₃ perovskite (Fe-free perovskite, or simply Pv) lies in a band in the lower part of the graph, whereas the two high-temperature ($T$ above 1000 K) measurements of $\alpha$ of Fe-rich perovskite, $(\text{Mg}_{0.9}\text{Fe}_{0.1})\text{SiO}_3$ (Fe-Pv), lie considerably higher on the graph. The dichotomy shown in Figure 1 is somewhat oversimplified because the experimental data in the lower band have different ranges of measurement. One curve in the lower band represents an extrapolation of data measured by Wang et al. (1994). Yet another curve in the lower band represents an independent theoretical calculation (for more details, see Fig. 1 caption). Nevertheless, Figure 1 correctly demonstrates the disparity between the high $\alpha(T)$ values held by one group of authors and the low $\alpha(T)$ values held by other groups of authors. At high $T$, Fe-Pv has an $\alpha$ value 1.5 times that of Pv. The Fe-Pv set of $\alpha$ curves produces a density profile at mantle conditions matching that of PREM, suggesting a chondritic-like lower mantle composition (Stixrude et al. 1992; Hemley et al. 1992; Jeanloz and Knittle 1989). The Pv $\alpha$ curves do not generate lower mantle density curves matching those of PREM, suggesting a pyrolitic composition (Jackson 1983; Wang et al. 1994; Zhao and Anderson 1994; Chopelas 1996; Jackson and Rigden 1996; Hama and Suito 1998). Such a large difference between these two sets of solutions for $\alpha$ was unexpected five years ago because values of the bulk modulus ($K_v$) and its pressure derivative ($K'_v$) were essentially the same for Fe-Pv as for Pv. This led to predictions that $\alpha$ would also not depend on Fe content, and therefore, future measured data on Pv $\alpha$ would converge with those on Fe-Pv $\alpha$ [in particular the upper curves in Fig. 1 (Jeanloz and Hemley 1994)]. As seen in Figure 1, high $T$ values of $\alpha$ found by recent measurements of MgSiO₃ do not converge with high $T$ values of $\alpha$ for Fe-Pv found by Mao et al. (1991) and Knittle et al. (1986), as Jeanloz and Hemley (1994) had predicted.

In an attempt to reconcile the data in Figure 1, it could be conjectured that the high $T$ values of $\alpha$ for Fe-Pv arise from the Fe itself (e.g., a considerable shift occurs in $\alpha$ with Fe content). A recent theoretical paper shows such a conjecture to be unfounded. Hama and Suito (1998), solving for thermoelastic constants using the Vinet equation of state, demonstrated that Fe-Pv and Pv yield virtually the same value of $\alpha$ at the $P$ and $T$ conditions of the lower mantle (see their Fig. 11). The data behind Figure 11 of Hama and Suito (1998) are listed in Table 1 here.

Thermodynamically, this study shows that the shift in $\alpha$ going from Pv to Fe-Pv is small by exploiting the properties of a Debye solid. MgSiO₃ perovskite has been proven to be a Debye-like solid by showing that using the Debye theory for Pv produces values of four thermoelastic parameters that agree with those measured or calculated by others (Anderson 1998). Further proof is shown in Table 2, which lists the values of $K'_v$ (isothermal bulk modulus), $K'_s$ (adiabatic bulk modulus), $v_s$ (longitudinal sound velocity), $v_p$ (shear velocity), and $\gamma$ (Grüneisen parameter), all vs. $T$, from both the Anderson (1998) Debye calculation and the Hama and Suito (1998) calculation. This table shows general agreement between the results from the Debye model and those from the theory based on the Vinet equation of state. The calculated volumetric thermal expansion of Fe-Pv $\alpha$ data is in good agreement with those measured for Fe-Pv.