Equation of state of MgSiO₃ with the perovskite structure based on experimental measurement

SURENDRA K. SAXENA,^{1,*} LEONID S. DUBROVINSKY,¹ FARAMARZ TUTTI,¹ AND TRISTAN LE BIHAN²

¹Department of Earth Sciences, Uppsala University, S-752 36 Uppsala, Sweden ²European Synchrotron Radiation Facility, BP 220, 38043 Grenoble, Cedex, France

Abstract

We studied MgSiO₃ with the perovskite structure heated to temperatures up to 1500 Kat pressures between 36 and 110 GPa with in-situ X-ray diffraction. The new pressurevolume-temperature (P-V-T) data were combined with literature data to provide thermal expansivity α and compressibility β against T (in K): $\alpha_T = 2.71 \times 10^{-5} + 1.80 \times 10^{-9} T$ $-1.48 T^2$ (Model 1) or $\alpha_T = 2.13 \times 10^{-5} + 7.57 \times 10^{-9} T - 1.02 T^2$ (Model 2), and β_T $= 3.735 \times 10^{-7} + 3.27 \times 10^{-11} T + 6.60 \times 10^{-15} T^2$. Model 1 yields physical properties of perovskite that confirm Anderson's (1998) Debye approach; the model is valid for extrapolation to 3000 K or more. The parameters at 300 K are: $\alpha = 1.1 \times 10^{-5}$, K_0 (bulk modulus) = 261 GPa, $K_0' = 4$ and $(\partial K/\partial T)_p = -0.027$. Thermal expansivity from this model does not fit the data of Funamori et al. (1996) at high temperature for P = 25 GPa. Model 2 uses an equation for α based on the data of Funamori et al. (1996), fits the available experimental data closely, and maintains conformity with Anderson's Debye approach. Heat capacity, C_{P} data for perovskite is given by either: $C_{P} = 110.8 + 8.031 \times$ $10^{-3} T - 1.302 \times 10^{-7} T^2 - 1.647 \times 10^7 T^2 + 2.755 \times 10^9 T^{-3} + 267.5 T^{-0.5} + 9287$ T^{-1} (Model 1) or $C_P = 121.33 + 2.77 \times 10^{-3} T - 2.585 \times 10^{-6} T^2 - 1.710 \times 10^{7} T + 10^{7} T +$ $2.792 \times 10^9 T^{-3} - 169 T^{-0.5} + 15782 T^{-1}$ (Model 2).