Thermoelastic properties of MgSiO₃ perovskite using the Debye approach

ORSON L. ANDERSON

Center for Physics and Chemistry of Planets, Institute of Geophysics and Planetary Physics, Department of Earth and Space Sciences, University of California at Los Angeles, Los Angeles, California 90095-1567, U.S.A.

Abstract

 $MgSiO_3$ perovskite is shown to be a Debye-like mineral by the determination of specific heat, $C_{\rm v}$, entropy, S, and thermal pressure, $\Delta P_{\rm Th}$, using the Debye theory up to 1800 K. Sound velocities and bulk moduli at ambient conditions published by Yeganeh-Haeri were used to find the ambient acoustic Debye temperature, Θ_{nc}^{∞} . The variation of Θ_{nc}^{∞} with T was assumed to be a curve parallel to the $\Theta_{\rm D}^{\rm ac}$ vs. T curves previously found for Al₂O₃, MgO, and MgSiO₃, enabling $\Theta_{\rm pc}^{\rm ac}(T)$ to be given up to 1800 K. To determine $C_{\rm P}$, the thermal expansivity, α , and the isothermal bulk modulus, $K_{\rm T}$, are needed. After considering several sets of $\alpha(T)$, the $\alpha(T)$ data of Funamori and his colleagues were chosen. Using the ambient K_{τ} and the values of $(\partial K_{\tau}/\partial T)_{P}$ vs. T reported by Jackson and Rigden, $K_{\tau}(T)$ up to 1800 K was found. Then $C_{\rm p}(T)$ up to 1800 K was found assuming quasiharmonicity in $C_{\rm v}$. The data behind the $C_{\rm p}(T)$ calculation are also sufficient to find the Grüneisen parameter, $\gamma(T)$, and the Anderson-Grüneisen parameters, δ_{τ} and δ_{s} , up to 1800 K. The value of $q = (\partial \ln \alpha)$ $\gamma/\partial \ln V$ _T was found, and with γ and ρ , ΔP_{Th} vs. V and T was determined. The three sound velocities, v_s , v_p , and $v_b = \sqrt{K_s/\rho}$, were then determined to 1800 K. From v_s and v_p , Poisson's ratio and the isotropic shear modulus, G, were found to 1800 K. MgSiO₃ perovskite is one of a small, select group of Debye-like minerals for which thermoelastic properties and the equation of state (EOS) are calculable from acoustic data.