Thermoelastic properties of MgSiO₃ perovskite using the Debye approach

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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 $\Theta_{\rm pc}^{\rm m}(T)$ 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.