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Thermoelastic properties of $MgSiO_3$ 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_V, entropy, S, and thermal pressure, ΔP_{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_D^{ac}. The variation of Θ_D^{ac} with T was assumed to be a curve parallel to the Θ_D^{ac} vs. T curves previously found for Al_2O_3, MgO, and $MgSiO_3$, enabling $\Theta_D^{ac}(T)$ to be given up to 1800 K. To determine C_P, the thermal expansivity, α, and the isothermal bulk modulus, K_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_T and the values of $(\partial K_T/\partial T)_P$ vs. T reported by Jackson and Rigden, $K_T(T)$ up to 1800 K was found. Then $C_P(T)$ up to 1800 K was found assuming quasiharmonicity in C_V. The data behind the $C_P(T)$ calculation are also sufficient to find the Grüneisen parameter, $\gamma(T)$, and the Anderson-Grüneisen parameters, δ_T and δ_S, up to 1800 K. The value of $q = (\partial \ln \gamma/\partial \ln V)_T$ 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. $MgSiO_3$ 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.