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Harmonic and anharmonic properties of spinel $MgAl_2O_4$

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ABSTRACT

The resonant sphere technique, RST, was applied to measure the elastic moduli of spinel. Resonant frequencies of 23 modes were measured between 293 and 1167 K. Results are similar to previous measurements by two of the authors (IS and OLA) using a rectangular prism specimen in that resonant frequencies of all modes decrease with temperature, and some modes show discontinuous change of slopes near 904 K. In the present work, inversion calculations of the frequency data to obtain elastic moduli was repeated until the standard error, σ, was minimized so that $\sigma = 0.16$ kHz (0.012%). Elastic moduli and their probable errors in GPa are: $C_{11} = 281.310 \pm 0.014$, $C_{12} = 155.437 \pm 0.013$, $C_{44} = 154.587 \pm 0.007$, and $C_s = 62.936 \pm 0.003$, where density $\rho = 3.5846$ g/cm^3 at 293 K. The anisotropy factor is $A = C_{44}/C_s = 2.46$ and is much larger than that of other cubic crystals. Isotropic properties are: bulk moduli, $K_S = 197.39 \pm 0.01$ GPa; isothermal bulk modulus, $K_T = 196.20$ GPa; and rigidity modulus, $\mu = 107.81$ GPa (the Hill average).

Temperature dependence was clarified for elastic moduli in which one of shear moduli, C_s [= $(C_{11} - C_{12})/2$] shows a distinctive bend at $T_c = 904$ K. The bend in K_S [= $(C_{11} + 2C_{12})/3$] at T_c is less pronounced because of opposite changes of slopes for C_{11} and C_{12} at 904 K. Combining elasticity and thermal expansivity data, we evaluate anharmonic parameters, resulting in the Grüneisen parameter, $\gamma = 1.17$, and the Anderson-Grüneisen parameters, $\delta_S = 2.98$ and $\delta_T = 4.72$ at $T = 300$ K; whereas, these are parameters are 1.10, 4.46, and 6.37, respectively, at $T = 1200$ K. The Grüneisen parameter is about 0.1 lower on the high-temperature side of T_c compared to its value on the low-temperature side.