American Mineralogist, Volume 86, pages 1188–1208, 2001

Thermal conductivity of spinels and olivines from vibrational spectroscopy: Ambient conditions

A.M. HOFMEISTER*

Department of Earth and Planetary Sciences, Washington University, St. Louis, Missouri 63130, U.S.A.

ABSTRACT

The damped harmonic oscillator model for thermal conductivity of insulators is improved, leading to a formula that predicts thermal conductivity at ambient conditions (k_0) from various physical properties, most of which are commonly measured. Specifically, $k_0 = [\rho/(3ZM)]\ C_V\ [(u_P + u_S)/2]^2/<\Gamma>$, where ρ is density, Z is the number of formula units in the primitive unit cell, M is the molar weight, C_V is heat capacity, u is the sound speed (P denotes compression; S denotes shear), and $<\Gamma>$ is the average of the damping coefficients determined from peak widths in infrared reflectivity spectra, or from suitable Raman and Brillouin spectra. The classical physics and quantum-mechanical basis for this model is discussed, with emphasis on the effect of phonon-phonon interactions on mode properties. The calculated values of k_0 all lie within the experimental uncertainty of the measurements for all samples with the spinel or olivine structure examined by Horai (1971) with known or approximately correct chemical compositions. Other divergent measurements of k for $MgAl_2O_4$ are discounted for various reasons. Early studies of Fe-bearing spinels are not generally reliable, but rough estimates from the above equation are consistent with all data, and good agreement is obtained for samples such as $Mg_{0.5}Fe_{0.5}Al_2O_4$ and γ-Fe_2SiO_4 for which the previous authors obtained chemical data, and for which IR reflectivity data exist. The theory reproduces the measured dependence of k_0 on composition and structure. Anisotropy in k_0 results mainly from differences in lattice constants (j): the equation for olivine is $k_j/k_0 = (V^{1/3}/j)^{0.73}$ which predicts the ratios within 3%. For solid solutions between Fe and Mg, the model provides a non-linear dependence of k_0 on mol% Fe, with the damping coefficient being the key factor producing non-linearity. Predicted ambient values are 11.3 ± 0.4 W/m-K for γ-Mg_2SiO_4, 6.5 ± 0.7 W/m-K for γ-$Mg_{1.2}Fe_{0.8}SiO_4$, and 6.9 ± 0.3 W/m-K for β-Mg_2SiO_4. The high k_0 for ringwoodite suggests that heat in Earth's transition zone should be conducted twice as efficiently as in the adjacent upper and lower mantles: this discontinuous depth dependence of k could impact thermal models of conduction in subducting slabs and of mantle convection