American Mineralogist, Volume 86, pages 622–639, 2001

Evaluation of shear moduli and other properties of silicates with the spinel structure from IR spectroscopy

A.M. HOFMEISTER[1,*] AND H.K. MAO[2]

[1]Department of Earth and Planetary Sciences, Washington University, St. Louis, Missouri 63130, U.S.A.
[2]Geophysical Laboratory and Center for High Pressure Research, 5251 Broad Branch Road, N.W., Washington, D.C. 20015, U.S.A.

ABSTRACT

Vibrational spectra are used to determine key physical properties of phases thought to be important in Earth's transition zone. Single-crystal infrared (IR) reflectance spectra were measured for synthetic Mg, Fe, Ni, or Co-bearing silicates with the spinel structure. Peak parameters (frequency, damping coefficient, and oscillator strength) were determined for the fundamentals, and for overtones, up to 3rd order. On average, the frequencies and damping coefficients of the overtones are simple multiples of the corresponding parameters of the fundamental modes. Absorption spectra of thin films were measured at pressures (P) up to 370 kbar for γ-Mg_2SiO_4 and up to 200 kbar for γ-Fe_2SiO_4. Widths are nearly constant, but frequencies (ν_i) increase either linearly or quadratically with P. For weak peaks, the absorption widths have values close to their corresponding damping coefficients. For γ-Fe_2SiO_4, ambient IR data predict heat capacity ($C_V = 126 \pm 2.5$ J/mol·K), shear modulus ($G = 875 \pm 15$ kbar), and sound velocities ($u_P = 8.20 \pm 0.05$, $u_S = 4.25 \pm 0.06$ km/s) at 298 K; pressure data give $\partial G/\partial P = 0.06$, 0.44, or 0.91 if for the bulk modulus, $\partial K/\partial P = 5$, 4.5, or 4, respectively, and an average mode Grüneisen parameter of $\langle\gamma\rangle = 1.45 \pm 0.4$, which implies that thermal expansivity is $(21 \pm 1) \times 10^{-6}$/K. For γ-$Mg_{1.2}Fe_{0.8}SiO_4$, ambient IR data predict $G = 1120 \pm 50$ kbar, $u_P = 9.12 \pm 0.20$, and $u_S = 5.18 \pm 0.20$ km/s at 298 K, assuming that the frequency of the acoustic mode is 225 to 240 cm^{-1}. This calculation uses $K_S = 1995$ kbar, which was obtained from recent compression data by assuming $\partial K/\partial P = 4$. The above values provide a smooth quadratic dependence of K_S and G on Fe/(Fe + Mg). The trends suggest that $\partial K/\partial P$ remains at 4 whereas $\partial G/\partial P$ drops from ~1 to ~0.5 as Fe content increases in ringwoodite. Acoustic fundamentals or overtones were used successfully here to provide u, G, and their P and T derivatives for silicate spinels. This method should work for other simple structures, and may be generally applicable.