Experimental Determination of Single-crystal Elastic Constants of Magnesiowüstite (Mg,Fe)O

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Introduction

One-dimensional seismic Earth models such as the Preliminary Earth Reference Model (PREM) [1] show discontinuous jumps of about 4.5% in compressional velocity, 6.3% in shear velocity, and 8.8% in density at 670-km depth. At the pressure and temperature appropriate for this depth, $(Mg,Fe)_2SiO_4$ spinel (γ phase) dissociates into $(Mg,Fe)SiO_3$ in the perovskite structure and magnesiowüstite (Mg,Fe)O [2, 3]. It has been proposed that that the mantle is chemically stratified, and an increase in silica and/or iron in the lower mantle adds to this discontinuity and may inhibit whole mantle convection. The three phases in question are solid solutions between magnesium and iron end-members, and their elastic properties are a function of pressure, temperature, and iron content. The discussion of whether or not the mantle is chemically stratified involves matching compressional and shear velocities, densities, and adiabatic bulk and shear moduli from seismic Earth models to mantle mineral assemblages. Magnesiowüstite is presumed to be the second-most-abundant mineral in the lower mantle, behind silicon-magnesium perovskite [2, 3]. A series of experiments carried out at GeoSoilEnviro (GSE)-CARS sector 13 explored the elasticity of magnesiowüstite as a function of pressure and iron content.

Methods and Materials

Polycrystalline $(Mg_{0.25},Fe_{0.75})O$ and $(Mg_{0.60},Fe_{0.40})O$ were provided by E. K. Graham at Pennsylvania State University. These were compressed in a diamond anvil cell to 46 GPa, with the compression axis perpendicular to the incident x-ray beam. The sample was held between the anvils with an x-ray transparent boron-epoxy gasket. The monochromatic beam was delivered at GSECARS beamlines 13-ID-D and 13-BM-D. Diffraction patterns were collected with a Bruker charge-coupled device (CCD) area detector, and raw data were analyzed by using the FIT2D program written by A. P. Hammersley from the European Synchrotron Radiation Facility.

Diffraction patterns were at every 3° between the maximum and minimum stress directions (Ψ = 0°-90°) for the 111, 200, 220, 311, and 222 reflecting planes. The compression was split into a hydrostatic component and deviatoric components by using Singh's model [4-6]:

$$d(hkl) = d_p(hkl)\{1 + \{1 - 3COS^2(\Psi)[Q(hkl)]\}\} ,$$

where $d_p(hkl)$ is the hydrostatic d-spacing and Q(hkl) is defined by $m_0 + m_1\Gamma(hkl)$ for the cubic system. $\Gamma(hkl)$ is a geometric quantity relating the particular reflecting plane:

$$\Gamma(hkl) = (h^2k^2 + k^2l^2 + l^2h^2)/(h^2 + k^2 + l^2)^2,$$

where $m_0 = (t/3)(S_{11} - S_{12})$ and where $m_1 = (-t/3)(S_{11} - S_{12} - S_{44}/2)$. Here S_{xx} represents components of the elastic compliance tensor, and t is the uniaxial stress component. The components of the elastic stiffness tensor are then computed from:

$$C_{11} = (1/3X) + (2t/9m_0),$$
$$C_{12} = (1/3X) - (t/9m_0), \text{ and}$$
$$C_{44} = t/[6(m_0m_1)],$$

where X = 1/3K is a measure of linear compressibility.

Results

Isothermal bulk and shear moduli were calculated from the resulting elastic tensors.

$(Mg_{0.6},Fe_{0.4})O$:

$K_T = 156.9 + 3.99P$ R = 0.999
$G = 70.95 + 0.712P$ R = 0.970

$(Mg_{0.25},Fe_{0.75})O$:

$K_T = 155.9 + 3.93P$ R = 0.999
$G = 70.74 + 0.50P$ R = 0.894

It is evident that iron has a greater effect on the shear modulus at lower mantle pressures.

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