Determination of elastic constants for MgO by means of high-resolution inelastic X-ray scattering

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The elastic properties of high-pressure minerals under their stable conditions are important information to estimate the structure of the Earth's interior. The technique of high-resolution inelastic X-ray scattering can provide the information even for opaque minerals. We performed this type of measurement on an MgO single crystal to estimate the elastic constants.

The sample was a commercial single crystal. The crystal orientation was determined by an X-ray Laue camera in our laboratory and cut into a appropriate shape. The experiment was performed at a high-resolution inelastic X-ray scattering beamline, BL35XU of SPring-8. The incident X ray was monochromatized with energy resolution of 1.5 meV. The scattered X-rays with 21.747-keV energy were acquired. The inelastic spectra were acquired along with reciprocal space directions of 400 to 500, 400 to 410 and 2-20 to 3-10.

The sound velocity is estimated from the value of E/k near gamma point, where E and k is the energy and crystal momentum of the phonon, respectively. We tried to calculate the elastic constants assuming that the phonon energy should be proportional to the crystal momentum. 34 data points, momentum transfer of which are almost perpendicular to reciprocal vectors of 100 or 110, are used for calculation. Obtained values are 309(11), 146(3), and 118(24) GPa for C_{11}, C_{44}, and C_{12}, respectively. The reliability factor of the least square fitting is 2.49%. The reported values are 297.8, 155.8, and 95.1 GPa for C_{11}, C_{44}, and C_{12}, respectively [1]. All values are consistent. The large errors are probably because the linearity between E and k is not a good approximation especially for C_{12}. The lattice dynamics model with a dynamical matrix is required for more accurate analysis. We would like to discuss the accuracy of this technique to estimate sound velocities more detail.

[1] Yoneda (1990) J. Phys. Earth **38**, 19-55