Dynamical lattice properties of $MgSiO_3$ perovskite at high pressure

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The Earth's lower mantle represents roughly the 60% of the Earth volume and principally consists of magnesium silicate with Fe and Al as minor elements [1]. At those depths, pressure lies between 24 and 110 GPa and this mineral assumes the perovskite form. Accordingly, $MgSiO_3$ magnesium perovskite can be considered as the most abundant mineral on the Earth. Unfortunately, its unstability at ambient condions delayed its discovery, irrespectively of its abundance [2].

The determination of the physical properties of magnesium perovskite is of fundamental geophysical interest. The mineral's equation of state and its elastic and thermodynamic properties at the relevant conditions of pressure and temperature are necessary for the interpretation of the preliminary reference Earth model and seismic tomography and to produce convection and mantle adiabatic models, which so far have been largely derived by calculations.

From the experimental standpoint, structural studies at extreme conditions have been extensively performed by X-ray diffraction on samples compressed in laser-heated diamond anvil cells [3], the elasticity tensor of $MgSiO_3$ perovskite at ambient conditions has been determined from measurements on both single-crystal and polycrystalline samples [4] and the aggregate shear modulus has been measured up to 96 GPa[5]. Despite the aboundance of structural experimental studies, the dynamics is still almost unexplored. An experimental phonon dispersion study to test the accuracy of lattice dynamics calculations at extreme conditions is indeed still missing.

The absence, up to now, of single crystal of good quality plagued these experimental studies. Very recently we succeded in obtaining good sub millimetric size single crystals perfectly adapted to be investigated in dimond anvil cell (DACs) by inelastic X-ray scattering (IXS) with meV energy resolution. Thus enabling combined pressure-temperature studies at several tents of GPa in pressure and temperatures up to 1100 K.

Within this contexct we started by investigating the phonon dispersion of single crystal $MgSiO_3$ along the main symmetry directions at ambient conditions and compared the excitation spectra with computed scattering intensities, which allow the validation of both calculated eigenvalues and eigenvectors [6].

Here we present a step forward of this combined study performed at the pertinent high-pressure conditions for the physical properties and chemical composition of Earth's lower mantle. Our results allow to extend the validity of the computational methods that in turn are used to derive the relevant thermodynamic and elastic properties at higher temperatures and pressures.

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