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Properties and phase relations of Wadsleyite II phase from first principles study

Kamil Tokar

Institute of Nuclear Physics, Polish Academy of Sciences, Material Research by Computers, Cracow, Poland (tokar@wolf.ifj.edu.pl)

Wadsleyite II is a magnesium-iron silicate phase similar to spinelloid IV and a potential host for hydrogen in the Transition Zone, between the wadsleyite and ringwoodite zones. There is a possibility that presence of this phase in the mantle could serve to obscure the transition at 525 km. It is clearly a new experimentally observed structure, although one very closely related to that of wadsleyite. The lattice of wadsleyite II is an orthorhombic, body-centered cell with I*mm*a space group. The unit cell parameters a,c are close to wadsleyite structure while b is 2.5 times larger than b in wadsleyite. Wadsleyite II, has one fifth of Si atoms in isolated tetrahedra and four fifths in Si_2O_7 groups as is typical for spinelloids IV. The sites of these groups in the crystal represent highly distorted tetrahedra with very long distance between Si and bridging oxygen atom.

The structure and stability properties of Mg_2SiO_4 wadsleyite II-phase have been studied from the first principles by application of the DFT+GGA method using PAW pseudo-potentials. Optimization procedures have been performed at hydrostatic pressures corresponding to the Transition Zone at the approximate depth of 525 km. The elasticity tensor coefficients C_{ij}(P) as well as Birch-Murnaghan equation of state for wadsleyite II structure have been determined from static calculations for external pressures up to 25 GPa. The aggregate compressional and shear wave velocities and their pressure derivatives have been also determined from these elastic properties. The lattice dynamics has been investigated by direct method and the thermodynamic model has been constructed using Quasi Harmonic Approximation (QHA). Raman frequencies and their symmetries have been derived at Gamma point of Brillouin zone. The stability of the crystal structure has been checked using dispersion curves plotted in directions connecting high symmetry points in reciprocal space and also from integrated phonon density of states (PDOS).

Thermodynamic properties like thermal expansivity, isothermal bulk modulus, entropy, specific heat capacity and thermal Grueneisen parameter have been derived from thermodynamic potentials in the validity range of QHA. Phase equilibria boundaries in Mg_2SiO_4 system have been constrained between wadsleyite II, wadsleyite and ringwoodite phases and studied in high pressure part of p-T diagram using thermodynamic method.