

THERMODYNAMIC ASSESSMENT OF THE MAGNESIUM-OLIVINE-PYROXENE SYSTEM USING A LATTICE VIBRATIONAL TECHNIQUE

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Phase diagrams are indispensable tools to provide geologists thermobarometric constraints in geological settings. Additionally thermophysical and thermochemical properties associated with the phases of materials in the phase diagram may be combined with seismological data to provide constraints on the overall composition and temperature of the Earth's mantle (Mattern et al. [1], Trampert et al. [2]).

We are currently constructing a thermodynamic database providing thermophysical and thermochemical properties and phase diagrams for materials with a geophysical relevance, applicable in the pressure and temperature regime of the Earth's mantle. The computational framework, which uses the thermodynamic database as input, is a combination between quantum mechanics and thermodynamics, allowing the calculation of longitudinal and transverse sound wave velocities enhancing the applicability to seismology. The computational technique is based on an extended form of Kieffer's [3] approach to model the vibrational density of states of a substance, a key property to derive the Helmholtz energy. The developed thermodynamic framework, which uses input parameters related to Raman and infrared spectroscopic data, puts tighter constraints on thermodynamic properties compared to methods based on polynomial parameterisations of thermal expansivity, heat capacity and isothermal bulk modulus. As shown by Jacobs and de Jong [4] and Jacobs et al. [5], this framework entails a description of thermodynamic properties free from physical anomalies for close-packed materials. In addition it discriminates, based on internal consistency, between the quality of disparate sets of experimental thermochemical, thermophysical and phase diagram data.

The present work focuses on the application of vibrational modeling to the magnesium-olivine-pyroxene system, which constitutes over 90% of the Earth's mantle and which is intimately linked to the magnesium-olivine system by the common phases wadsleyite, ringwoodite and perovskite. We show how our approach is used in a thermodynamic assessment of experimental data and compare the results with those obtained from ab-initio calculations. The results, which will be presented here, were used in a numerical model of convection in the Earth's mantle to reveal, among other things, effects of phase transitions on the degree of layering, mineral distribution and sound wave velocities in the transition zone, around 660 km depth in the Earth.

References

- [1] E. Mattern, J. Matas, Y. Ricard and J. Bass, *Geophys. J. Int.*, **160**, 973-990 (2005)
- [2] J. Trampert, P. Vacher and N.J. Vlaar, *Phys. Earth Plan. Inter.*, **124**, 255-267 (2001)
- [3] S.W. Kieffer, *Rev. Geophys. Space Physics*, **17**, 35-59 (1979)
- [4] M.H.G. Jacobs and B.H.W.S. de Jong, *Phys. Chem. Minerals*, **32**, 614-626 (2005)
- [5] M.H.G. Jacobs, A.P. van den Berg and B.H.W.S. de Jong, *Calphad*, in press (2006)