Thermodynamic assessment of the magnesium-olivine-pyroxene system using a lattice vibrational technique

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We are currently constructing a thermodynamic database providing phase diagrams, thermophysical and thermochemical properties for materials with a geophysical relevance, applicable in the pressure and temperature regime of the Earth's mantle. The computational technique is based on Kieffer's (1979) approach to model the vibrational density of states of a substance, a key property to derive the Helmholtz energy. It allows the calculation of V_P and V_S sound wave velocities. The developed thermodynamic framework uses model input properties related to Raman and infrared spectroscopic data. It puts tighter constraints on thermodynamic properties compared to methods based on polynomial parameterisations of thermal expansivity, heat capacity and isothermal bulk modulus. Jacobs and de Jong (2005) and Jacobs *et al*. (2006), showed that this framework entails a description of 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. The results, presented here, were used in a numerical model of convection in the Earth's mantle to reveal, 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.

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Accretion and early differentiation history of the Earth based on extinct and long-lived chronometers

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Jacobsen and Harper (1996) showed that isotopic variations due to decay of extinct nuclides (^{129}I, ^{244}Pu, ^{182}Hf and ^{146}Sm) could be used to study early evolution of terrestrial reservoirs and provide observational constraints on the timescale of accretion of the terrestrial planets. Measurable variations in ^{182}W/^{183}W, ^{142}Nd/^{144}Nd, ^{129}Xe/^{130}Xe and ^{136}XePu/^{130}Xe in the Earth (compared to bulk planetary values inferred from primitive meteorites) provide a preserved record of accretion, core formation, early crust, atmosphere formation and evolution. The ^{182}Hf-^{182}W system is the best accretion and core-formation chronometer because it is identifiable with chemical fractionation during the accretion process itself. This system yields a mean time of Earth's accretion and core formation of 10 Myr, with a total timescale of accretion being 30 Myr. New experimental data pertaining to the conditions that existed in the Earths deep mantle (P > 100 GPa and T > 6000 K) subsequent to the giant Moon-forming impact show that metal-silicate equilibration will be rapid enough for the Hf-W chronometer to reliably record this timescale (Petaev *et al.* 2007). Although the ^{207}Pb-^{206}Pb chronometer has been used to argue for a more protracted timescale (~100 Myr) of accretion and core formation, Yin and Jacobsen (2006) showed that these data do not require a longer time scale. Using the coupled ^{146}Sm - ^{147}Sm chronometer, the age of the initial silicate differentiation in the mantle source region of some of the Earth's oldest surviving crustal rocks can be constrained to ~4.47 Ga. Attempts to use this chronometer for dating proto-crust formation at ~30 Myr are unreliable because of the uncertainties in the initial Nd isotopic composition inferred from heterogeneities in Ba and Nd isotopes in primitive meteorites (Ranen and Jacobsen 2006). The presence of a large ^{129}Xe excess in the deep Earth is consistent with a very early formation and a short time interval for the accretion of the Earth.

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