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A thermodynamic recipe for baking the Earth's lower mantle and core as a whole

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A rigorous understanding of the thermal and dynamic evolution of the core and the interaction with the silicate mantle cannot preclude a non-empirical petrological description of the problem which takes the form of a thermodynamic model. Because the Earth's core is predominantly made of iron such model may seem relatively straightforward, simply delivering a representation of the phase transformations in the P,T space. However due to well known geophysical considerations, a certain amount of light elements should be added. With the Occam's razor principle in mind, potential candidates could be the most abundant and easily accessible elements in the mantle, O, Si and Mg. Given these premises, the challenging problems on developing this type of model are:

- a thermodynamic formulation should not simply describe phase equilibrium relations at least in the Fe-Si-O system (a formidable task itself) but should be also consistently applicable to evaluate thermophysical properties of liquid components and solids phases at extreme conditions (P=500-2000 kbar, T=1000-5000 K). Presently these properties are unknown for certain mineral and liquid components or partially available from scattered sources.
- experimental data on the phase relations for iron rich liquid are extremely difficult to obtain and could not cover the entire P,T,X spectrum.
- interaction of the outer core with the silicate mantle requires a melt model that is capable of describing a vast range of compositions ranging from metal-rich liquids to silicate liquids.

The compound energy formalism for liquids with variable tendency to ionization developed by Hillert and coworkers is a sublattice model with varying stoichiometry that includes vacancies and neutral species in one site. It represents the ideal candidate for the task in hand. The thermodynamic model unfortunately is rather complex and a detailed description of the formulation for practical applications like chemical equilibrium calculations is nowhere to be found, while the model is only accessible on few commercial thermodynamic programs.

The latest developments regarding all these related issues will be discussed in this contribution. In particular some self-consistent but preliminary results will be presented addressing the following topics:

- some details regarding the implementation of the liquid model for Gibbs free energy minimizations,
- the physically consistent behavior of thermodynamic properties of certain solid phases like (Fe,O,Si) BCC, FCC, HCP and liquid components,
- selected phase diagrams at core conditions in the system Fe-Si-O,
- derived geotherms linking the inner-outer core with the core-mantle boundary.
- brief outline of the future geodynamic applications.