Geophysical Research Abstracts,
Vol. 10, EGU2008-A-05921, 2008
SRef-ID: 1607-7962/gra/EGU2008-A-05921
EGU General Assembly 2008
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PreMDB, a thermodynamically consistent material database as a key to geodynamic modelling

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The Preliminary Reference Earth Material DataBase (PreMDB) is a new tool for coupling thermochemistry with mechanics. The main purpose of PreMDB is to provide modellers with a complete and easy access to fundamental material data for terrestrial rocks and minerals. Another goal is to standardise material data to compare results from various numerical and experimental techniques. Currently, PreMDB lists 47 major rock forming dry and wet minerals and 10 terrestrial rocks, representing a standard for marine sediments [1], the upper and lower continental crust [2, 3], oceanic crust [4] and mantle (pyrolite and peridotite) [5, 6]. For each rock and mineral, 20 thermodynamic, thermal, elastic, seismic and mechanical properties are defined between 0.05-5 GPa and 400-1600K.

Recent studies [7, 8] have shown that physical properties of terrestrial rocks and minerals derived from thermodynamic potentials provide an important complement to geophysical observations and experimental measurements. Properties previously determined from laboratory analyses can now be derived self-consistently from thermodynamic modelling for the full temperature and pressure range in the earth's interior. Thermodynamic potential functions are thus used to calculate reversible material prop-

erties such as thermal expansion coefficient, specific heat, elastic shear modulus, bulk modulus and density. Subsequently, thermodynamic potential functions can be used to drive geodynamical processes by solving the heat equation without applying external boundary conditions. Specifically, density differences driving for instance subduction do not need to be assigned but they follow from chemical composition and temperature.

We chose the Gibbs energy minimisation algorithm Perple_X to compute phase equilibria, maps phase relations and extracts mineral physical properties of geodynamical interest. Perple_X is robust and computes stable mineral assemblages. In particular, Perple_X predicts phase transitions that are important for seismic tomography and geodynamic modelling. Moreover, in contrast to codes using non-linear techniques for Gibbs energy minimisation (ThermoCalc, Domino, FreeGs), Perple_X utilises a linearized formulation of the minimisation problem which always converges and minimizes data gaps.

Transport properties such as thermal conductivity (diffusivity) and melt viscosity are also included, but these are derived from laboratory experiments. These properties are included to provide a reference database as a common standard of material properties necessary for performing realistic simulations of rock behaviour during geological and geodynamic processes.

The model fits the PREM and ak135 seismic models and may even record more precise discontinuities due to thermodynamically predicted phase transitions. Density, P- and S-wave velocity and Poisson's ratio simulated for pyrolitic compositions with varying Al_2O_3, CaO and FeO contents show global agreement with the seismological data down to the core-mantle boundary. The autocorrelation functions respectively vary between 0.996-0.998, 0.996-0.998, 0.988-0.995 and 0.748-0.779 for PreMDB/PREM and 0.992-0.996, 0.994-0.997, 0.987-0.994 and 0.763-0783 for PreMDB/ak135. The discrepancy for the Poisson's ratio results from the square root relation between the P- and S-wave velocity ratio and the Poisson's ratio, making this parameter more sensitive to chemistry. This result suggests that the Poisson's ratio is a useful marker of the variation of mantle composition with depth and may be used for future fine tuning of mantle chemistry.

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