



Deep mantle melting-solidifying and produced heterogeneities

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Model for solid-liquid equilibrium and substance properties in lower mantle conditions is important to understand the early stages of evolution of terrestrial planets, such as core formation and magma ocean crystallization. This model is also necessary to prove theories on some modern seismic features of the Earth (e.g. ultra-low velocity zones) and petrological observations (e.g. lower mantle mineral assemblage inclusions in diamonds).

Numerous experimental and numerical studies of the lower mantle phases provide sufficient amount of data to build up a thermodynamic model, which can be used in geophysical fluid dynamics research. Molecular Dynamics modeling provides data on thermodynamic properties of solids and liquids (density, heat capacity, thermal expansion, latent heat of melting etc.). Absence of minor components (iron, alkali etc.) makes it to overestimate melting temperatures significantly (up to 20-30%), so experimental data are also very important.

Our model is based on MD data by [de Koker et al., 2013] with evaluation of all important parameters according to classical thermodynamic equations. Melting temperatures (especially at eutectic points) are corrected along Clausius-Clapeyron slopes to agree with modern experimental data ([Andraut et al., 2011], [Andraut et al., 2014], [Fiquet et al., 2010], [Hirose et al., 1999], [Mosenfelder et al., 2007], [Nomura et al., 2014], [Ozawa et al., 2011], [Zerr et al., 1998]). KD value for iron reported by [Andraut et al., 2012] was used.

Proposed model was implemented into StagYY software (e.g. [Tackley, 2008]). It is a finite-volume discretization code for advection of solid and liquid in a planetary scale. A principal new feature of the used code modification is that we use separated variables for chemical compounds: SiO₂, FeO, MgO and other (list can be extended). So it is possible to trace mantle heterogeneities produced by melting and solidifying events.

Calculations predict appearing and disappearing batches containing up to 5-7% of melt (CMB temperature 4000-4400 K). Amount of FeO in liquid is up to 18%, so melts are 2 % denser than solid counterpart, resulting in total density increase up to 1 %. This data fits properties proposed for Ultra-Low Velocity Zones (melt fraction between 5 and 30 % [Garnero et al., 1998], and density increase of at least 1% [Beuchert & Schmeling, 2013]).