



The effect of iron spin transition on convective dynamics, slab dynamics and the geoid

Michael Jacobs (1), Arie van den Berg (2), Wim Spakman (2), Ondrej Cadek (3), Hana Cizkova (3), and Ctirad Matyska (3)

(1) Institute of Metallurgy, TU-Clausthal, Clausthal-Zellerfeld, Germany, (2) Institute of Earth Sciences, Utrecht University, Utrecht, The Netherlands, (3) Department of Geophysics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

Iron bearing minerals in the Earth's lower mantle show a transition from high-spin to low-spin in the iron constituent. This has been observed in particular for ferropericlase both experimentally (Fei et al, 2007, Lin et al. 2005) and in first principles calculations (Wu et al, 2009). The situation is less unambiguous for perovskite. Umemoto et al (2010) showed that the effect on volume is small compared to experimental uncertainty. Therefore we only considered the spin effects in ferropericlase in our models.

The spin transition is characterized by a high valued positive Clapeyron slope $\gamma = 19 \text{ MPa/K}$ while the smoothness of the transition increases with temperature. Fei et al. (2007) showed that at room temperature the spin transition pressure for iron richer composition occurs at higher values, e.g. 40 GPa at 20 mol% FeO, 60 GPa at 40 mol% FeO.

In order to get a full thermodynamic description of mantle material that includes the effects of spin transitions in ferropericlase we developed a model based on the multi-Einstein vibrational model approach of Jacobs et al. (2013). This model represents volume-pressure data of Lin et al. (2005), spin fraction data predicted by Wu et al. (2009) and it also includes the observed composition dependence of the spin transition pressure.

Our new model further includes the thermodynamic description of Jacobs and de Jong (2007) that has been extended to describe thermodynamic properties of iron bearing $(\text{Mg,Fe})\text{SiO}_3$ perovskite. Because the spin transition pressure is composition dependent, the spin transition results in the formation of miscibility gap regions separating compositions enriched in high spin and compositions enriched in low-spin state.

The spin transition affects thermodynamic properties, density, thermal expansivity, bulk modulus and heat capacity which in turn impact the convection dynamics of the Earth mantle. For instance, due to the high positive Clapeyron-slope of the transition convective mixing becomes more vigorous as observed in Boussinesq type modelling results of Bower et al, 2009, Shanas et al, 2011. Negative buoyancy of lithospheric slabs in the deep mantle is enhanced by the increase of thermal expansivity induced by the spin transition. Therefore the sinking rate of slabs are affected by the presence of the spin transition. Therefore the effects of the transition must be included in mantle convection modelling, done in order to bracket mantle viscosity values (Cizkova et al., 2012).

Here we investigate the impact of the iron spin transition on the convective dynamics of the mantle and the distribution of material properties. As the spin transition related variations of material properties (e.g. thermal expansivity) are significant especially at lower temperatures, we concentrate mainly on the consequences for slab dynamics. To this end we use a compressible convection model based on a self consistent formulation of the thermo-physical material properties density, thermal expansivity and specific heat at constant pressure as described in (Jacobs and van den Berg, 2011). Finally, we evaluate the consequences of spin induced density contrasts in cold downwellings for the interpretation of the geoid.

- Bower et al. (2009) *Geophys Res Lett*, 36, L10306
Cizkova et al. (2012) *Phys Earth Planet Inter* 200, 56-62
Fei et al. (2007) *Geophys res Lett*, 34, L17307, 1-5
Jacobs and de Jong (2007) *Geochim Cosmochim Acta*, 71, 3630-3655
Jacobs and van den Berg (2011) *Phys Earth Planet Inter*, 186, 36-48
Jacobs et al. (2013) *Phys Chem Minerals*, in press
Lin et al. (2005) *Nature* 436, 377-380
Shanas et al (2011) *J Geophys Res* 116, B08205, 1-16
Umemoto et al (2010) *Phys Earth Planet Int*, 180, 209-214
Wu et al (2009) *Phys Rev B* 80, 014409, 1-8