

## Nucleation and growth of calcite particles: Comparing modelling and experimental approaches

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The development of CO<sub>2</sub> storage projects stimulates an extensive use of geochemical models for the precipitation of mineral phases and particularly carbonate phases. A thorough modelling of the formation of secondary minerals in geochemical processes requires an account of nucleation and growth mechanisms in a generalized kinetic approach. We have developed the Nanokin code [1-3] which models kinetic dissolution of primary minerals and precipitation of secondary minerals, relating the nucleation and growth of precipitated particles to the saturation state of the aqueous solution. This model predicts the size evolution of created particles and the feedback effect on the aqueous composition.

We present an application of the Nanokin code to the formation of calcite from a supersaturated solution produced by the dissolution of portlandite at 30°C with a high pH value around 12. These conditions correspond to those selected by Montes *et al.* [4] in their recent experimental approach. The simulated calcite particles are produced by heterogeneous nucleation and tri-dimensional growth.

The results show that the nucleation of calcite occurs rapidly from the initial dissolution stages of portlandite as obtained experimentally during the first 5 hours of reaction. The nucleated particles grow over 24 hours, reaching sizes of about 70-75 nm which compare well to the sizes obtained experimentally (64 nm).

This modelling approach validated at 30°C may be extended to higher temperatures up to 90°C as in the experimental approach.

[1] B. Fritz, A. Clément, Y. Amal, & C. Noguera (2009) *GCA* **73**, 1340–1358. [2] Noguera C. Fritz B. Clément A. & Amal Y. (2010) *Chem Geol.* **269**, 89–99. [3] Noguera C. Fritz B. & Clément A. (2011) *GCA* (in press) DOI: 10.1016/j.gca.2011.03.016. [4] F. Montes-Hernandez, A. Fernandez-Martinez & F. Renard (2009) *Crystal Growth & Design* **9**(10), 4567–4573.

## Spin crossover and iron-rich silicate melt in the Earth's deep mantle

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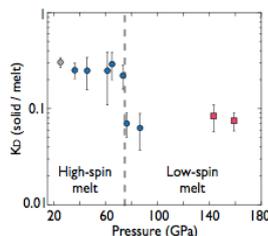
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The density crossover between melt and solid in the deep mantle has long been speculated with profound implications for chemical evolution of our planet[1]. Recent *ab-initio* calculations[2] suggested that melt-solid iron partitioning is the key to cause density crossover, which has been examined only at low pressures (25 GPa)[3].

In this study, we performed melting experiments on (Mg<sub>0.89</sub>Fe<sub>0.11</sub>)<sub>2</sub>SiO<sub>4</sub> olivine using laser-heated diamond anvil cell (LHDAC) and extended measurements of iron partitioning over the entire mantle pressure range.

The calculated Mg-Fe distribution coefficient  $K_D$  between melt and liquidus phase (Fig. 1) showed the sudden drop of  $K_D$  value at about 76 GPa, which could be explained by a Fe<sup>2+</sup> spin crossover (from high-spin to low-spin) in melt suggested by additional X-ray emission spectroscopy (XES) measurements in (Mg<sub>0.95</sub>Fe<sub>0.05</sub>)SiO<sub>3</sub> glass which observed the change of spin state at about 70 GPa and room temperature.

The calculated density of (Mg, Fe)SiO<sub>3</sub> liquid coexisting with (Mg<sub>0.92</sub>Fe<sub>0.08</sub>)SiO<sub>3</sub> perovskite shows that melt is denser than solid below 1800 km depth in the Earth. These results suggest that dense basal magma ocean in the early Earth whose subsequent crystallization may have formed large low shear velocity provinces (LLSVPs) and ultra low velocity zone (ULVZ).



**Figure 1:** Change in Fe-Mg distribution coefficient  $K_D$  between perovskite (blue circle) or post-perovskite (red square) and melt. The datum of previous experiment is shown in grey circle [3].

[1] Labrosse *et al.* (2007) *Nature* **450**, 866–869. [2] Stixrude *et al.* (2009) *EPSL* **278**, 226–232. [3] Corgne *et al.* (2005) *GCA* **69**, 485–496