

CO₂ speciation and transport properties of CO₂-bearing silicate melts from First-Principle simulations

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There are growing evidences of the existence of CO₂-rich magmas in the upper mantle [1-3]. So the role of carbon-rich melts at depth is now becoming a credible scenario to explain the extraction of CO₂ from the source region to the surface. During the last three decades many studies have been devoted to measure the solubility of CO₂ in silicate melts of various composition. But due to experimental difficulties these studies were generally restricted to low and moderate pressures (below ~20 kbar). IR spectroscopy has emphasized the importance of CO₂ speciation which may exist either as molecular CO₂ or as carbonate ion (CO₃²⁻), the molecular form being favored in polymerized (silicic) melts while the carbonate ion is dominant in depolymerized (basic and ultrabasic) melts. However it has been suggested recently [4,5] that the CO₂ speciation observed in quenched glasses by IR spectroscopy may not be representative of that in silicate melts equilibrated at high temperature.

To address this issue we have performed First-Principle Molecular Dynamics of CO₂-saturated basaltic and kimberlitic melts. The molecular form is indeed favored in the more polymerized melt. Furthermore, a new transient species is also identified. The electrical conductivity of the CO₂-saturated basaltic and kimberlitic melts has also been evaluated and found in good agreement with experiment. These results have also been used to develop an empirical force field for describing CO₂-rich melts by classical MD simulations.

[1] Dasgupta & Hirschmann (2007) *Nature* **440**, 659-662. [2] Zeng *et al.* (2010) *North China. Chem. Geol.* **273**, 35-45. [3] Helo *et al.* (2011) *Nature Geoscience* **4**, 260-263. [4] Morizet *et al.* (2007) *Eur. J. Mineral.* **19**, 657-669. [5] Spickenbom *et al.* (2010) *GCA* **74**, 6541-6564.

Microstructural control on trace element diffusion in pyrrhotite from komatiite hosted massive Ni sulphides, Yilgarn Craton

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Pyrrhotites (Fe₇S₈) from three different komatiite hosted massive nickel sulphide deposits have been analysed with electron backscatter diffraction analysis (EBSD) and laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) in order to understand how trace elements behave during deformation.

EBSD data reveals strain localisation microstructures in sample from greenschist facies whereas in sample from mid-amphibolite facies, pyrrhotite contains multiple parallel low angle boundaries and crystallographic preferred orientation. A sample from the upper amphibolite facies, is characterised by very large >2cm grains that contains numerous deformation twins. Laser ablation ICP-MS data reveal increased concentrations of Pb, Bi and Ag along low angle subgrain boundaries and twin boundaries. The increased concentrations of Pb, Bi and Ag are explained by diffusion of the trace elements along fast diffusion pathways (low angle and twin boundaries). Trace element variations are developed at the low-temperature stage of the tectonic history of the three deposits. Diffusion of Pb, Bi and Ag is triggered by their low solubility in sulphide phase, pyrrhotite.