Iron spin crossover in the new hexagonal aluminous (NAL) phase

HAN HSU

Department of Physics, National Central University, Taoyuan City 32001, Taiwan (hanhsu@ncu.edu.tw)

The new hexagonal aluminous (NAL) phase, chemical formula $AB_2C_6O_{12}$ (A = Na^+, K^+, Ca^{2+}; B = Mg^{2+}, Fe^{2+}, Fe^{3+}; C = Al^{3+}, Si^{4+}, Fe^{3+}), is considered a major component (~20 vol%) of mid-ocean ridge basalt (MORB) under the lower-mantle condition. As MORB can be transported back into the Earth's lower mantle via subduction, a thorough knowledge of the NAL phase is essential to fully understand the fate of subducted MORB and its role in mantle dynamics and heterogeneity. In this presentation, the complicated spin crossover of the Fe-bearing NAL phase will be discussed based on a series of first-principles calculations [1], in which the local density approximation + self-consistent Hubbard U (LDA+U_{sc}) method was adopted. As revealed by these calculations, only the ferric iron (Fe^{3+}) substituting Al/Si in the octahedral (C) site undergoes a crossover from the high-spin (HS) to the low-spin (LS) state at ~40 GPa, while iron substituting Mg in the trigonal-prismatic (B) site remains in the HS state, regardless of its oxidation state (Fe^{2+} or Fe^{3+}). The volume/elastic anomalies and the iron nuclear quadrupole splittings determined by calculations are in great agreement with room-temperature experiments [2]. The calculations further predict that the HS-LS transition pressure of the NAL phase barely increases with temperature due to the three nearly degenerate LS states of Fe^{3+}, suggesting that the elastic anomalies of this mineral can occur at the top lower mantle.

[1] Hsu (2017) *Phys. Rev. B* **95**, 020406(R). [2] Wu *et al.* (2016) *Earth Planet. Sci. Lett.* **434**, 91-100.