

Dynamical effect of the spin transition: A numerical simulation study

Taku Tsuchiya[1]; Jun Tsuchiya[2]

[1] GRC, Ehime Univ; [2] GRC, Ehime University

Recent studies suggest that the spin transition of iron in the mantle minerals can cause several new exotic phenomena, which might give important consequences on the mantle mineralogy. Theoretical free energy modelling combining with density functional computation proposed a broad pressure region where high-spin and low-spin iron coexist along the mantle geotherm. Across this high-spin/low-spin mixed state, any properties are expected to vary continuously. This transient behavior has been successfully confirmed experimentally. And more recently, surprising elastic softening has also been reported across the spin transition. However, the dynamical effect of the spin crossover is still little understood. In this study, we have performed thousands atom numerical simulations to model the mixed spin state. Calculations suggest important consequences that the spin transition is accompanied with anomalous behaviors driven by dynamical fluctuation of spin state, even though the structure remains macroscopically isosymmetric.

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