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第一原理計算から予測される鉄の乱層構造

Prediction of turbostratic iron from first-principles

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Determining the crystal structure of iron in the Earth's inner core has been a long standing challenge for mineral physics. The hexagonal close-packed (hcp) structure has been predicted to be a dominant candidate structure [1,2]. However, the double hcp structure [3], the face-centered cubic (fcc) structure [4], the body-centered cubic structure [5] have also been suggested and it is still controversial. Here we propose another model for the structure of iron at the extreme conditions. The model was predicted by structural exploration methods based on first-principles calculations, which are free energy surface trekking (FEST) and multiple-configuration sampling method (MCS) [6]. Exploring the metastable structures at 400 GPa by FEST, we found that the hcp iron transforms to a structure with complex stacking sequence by shear deformation and it is much more easily obtained from hcp than fcc. Based on the results of FEST, we inferred a stacking disorder structure stabilizing with a temperature-dependent stacking fault concentration, which we call turbostratic iron. Then, we determined the thermally-equilibrated stacking fault concentration at each temperature by the MCS method. At the moment, neglecting phonon contributions, we found that iron has the stacking fault concentration of about 8% at around 1000 K but it increases to about 40% at the inner core conditions. Then, we analyzed elastic properties of turbostratic iron and found that the stacking fault enhances elastic anisotropy. We anticipate that the model of the turbostratic iron gives some new aspects for the inner core structure.

Reference:
[1] Y. Z. Ma, M. Somayazulu, G. Shen, H. K. Mao, J. F. Shu, R. J. Hemley, Phys. Earth Planet. Inter. 143, 455 (2004).
[2] G. Steinle-Neumann, L. Stixrude, R. E. Cohen, O. Gulseren, Nature 413, 57 (2001).
[3] S. K. Saxena, L. S. Dubrovinsky, P. Haggkvist, Y. Cerenius, G. Shen, H. K. Mao, Science 269, 1703 (1995).
[4] A. S. Mikhaylushkin, S. I. Simak, L. Dubrovinskaia, B. Johansson, I. A. Abrikosov, Phys. Rev. Lett. 99, 165505 (2007).
[5] L. Vo?adlo, I. G. Wood, M. J. Gillan, J. Brodholt, D. P. Dobson, G. D. Price, D. Alfe, Phys. Earth Planet. Inter. 170, 52 (2008).
[6] J. Tsuchiya, T. Tsuchiya, Proc. Natl. Acad. Sci. USA 105, 19160 (2008).

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