First-principles Study on Crystal Structures of Calcium and Iron under High Pressure

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Calcium, an alkali earth metal, takes a face-centered cubic (fcc) structure (Ca-I) at ambient condition and it transforms to a body-centered cubic (bcc) structure (Ca-II) at 20GPa. The bcc structure transforms to a simple cubic structure (Ca-III) at 32GPa. By further compression, Ca-IV (113-137 GPa) and Ca-V (137 GPa-) emerge (T. Yabuuchi *et al.*, J. Phys. Soc. Jpn. **74**, 2391 (2005)), each of which has a complex crystal structure. Both Ca-IV and Ca-V have a coordination number of 7 and the structure of Ca-IV is a four-fold helical structure and that of Ca-V a zigzag structure (T. Ishikawa *et al.*, Phys. Rev. B **77**, 020101 (2008), Fujihisa *et al.*, Phys. Rev. Lett. **101**, 095503 (2008)). Instead of decreasing the electrons of 4s-character of calcium, those of 3d- are increased with pressure, which is called the s-d transfer. This result indicates that calcium behaves like a 3d transition metal in Ca-IV and Ca-V with the complex crystal structures. From this fact, there is the possibility that iron, which is the 3d transition metal and a primary constituent of the Earth's core, also takes complex crystal structures in high-pressure conditions. In this study, we explore the hypothesis using the complex crystal structures of calcium for iron and comparing the energy differences among the candidate structures.