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철의 결정구조와 스핀구조에 대한 제일원리 전산모사 연구

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1. 서 론

Due to the four unpaired valence electrons of its atom, Fe in its various forms (clusters, surfaces, thin films, and bulk) shows very rich magnetic phenomena. Many first-principles studies successfully described the magnetic phases of bulk and thin-film Fe. A number of earlier calculations employed the all-electron full potential linearized augmented plane-wave (FLAPW) DFT method. Here we have studied crystal and spin structures of iron with first-principles pseudo-potential methods.

2. 계산방법

The calculations are carried out using the density functional theory in the generalized gradient approximation, norm-conserving, non-local, scalar-relativistic pseudopotentials, and numerical double zeta plus polarization basis functions for 4s, 4p, and 3d of Fe. The spacing of the regular real space grid is determined by the maximum kinetic energy of the plane waves that can be still represented in the grid. We use here the cutoff value of 200 Ry.

3. 계산결과

Ab initio electronic-structure calculations, based on density-functional theory and a pseudo-potential method, have been used to predict crystal-structure phase stabilities. Total energies for four crystal structures, bcc, fcc, hcp, and dhcp, and five spin structures of ferromagnetic high-spin state and low-spin state, anti-ferromagnetic high & low spin states, and nonmagnetic state , have been calculated over a wide volume range. In agreement with experiment and previous theoretical calculations, a magnetic bcc ground state is obtained at ambient pressure and a nonmagnetic hcp ground state is found at high pressure, with a predicted bcc → hcp phase transition. Also a metastable dhcp phase is found at high pressure, which remains magnetic and consequently accessible at high temperature. In addition, the bcc structure becomes mechanically unstable at high pressures and a metastable, but still magnetic.