First-principles approach to theory of permanent magnets

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Due to increasing demand for motors and wind turbines, scarce-element-lean permanent magnets with enhanced performance have attracted much attention. One of the most important features dominating permanent-magnet performance is the microstructure, i.e., mesoscopic arrangements of multiple phases, because interfaces between constituent phases prevent the domain-wall motion that induces magnetization reversal. Thus, local magnetic anisotropy at interfaces is of importance on the atomic scale [1,2], where the crystal-field analysis for rare-earth 4f electrons is useful. On the mesoscopic scale, microstructures are determined by phase equilibria, where the Gibbs free energy is minimized. From this aspect, first-principles evaluation of the Gibbs energy is crucial, because full composition landscapes of Gibbs energies for various phases should be determined, many of which are unavailable by experiments. The Gibbs energy consists of the ground-state internal energy, the electronic free energy, the phonon free energy, the magnetic free energy, and the configurational-entropy term. Thus, even if magnetic phase transition is discussed, the minimization should be considered for the total free energy instead of the magnetic free energy. For example, since phonon frequencies of bcc Fe for the ferromagnetic state are higher than those for the paramagnetic state, magnetic phase stability is affected according to the minimization of the total free energy: This stabilization of the paramagnetic state lowers the theoretical Curie temperature by more than 500 K [3]. The same tendency is observed for $Nd_2Fe_{14}B$, the main-phase compound of the neodymium magnet [4]. Getting back on track of microstructures, phase equilibria between the main phase and subphases of the so-called 1-12 magnet are also discussed from first principles [5,6].

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