Electron theory of permanent magnets

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Man-made permanent magnets have a long history (over one hundred years). Magnetic steels, such as KS- and MK-steels, were the best magnets in the early 20th century. They were followed by alnico magnets (alloys made up of Al, Ni and Co) appeared in the 1930s. In the 1960s samarium cobalt magnets brought drastic increase in the maximum energy product $(BH)_{max}$, which is the figure of merit for permanent magnets. Subsequently, various types of rare-earth magnets have been invented. Among them, neodymium-iron-boron ($Nd_2Fe_{14}B$) has been the strongest one for thirty years.

The theoretical limit of $(BH)_{max}$ is given by $\mu_0 M_s^2/4$, where M_s is the saturation magnetization. It is achieved only when the coercivity is larger than $M_s/2$. Here the coercivity is the magnetic field at which magnetic reversal takes place, and it has correlation with the magnetic crystalline anisotropy energy. The magnetization and magnetic crystalline anisotropy energy are thus basic physical quantities to characterize hard magnet. The Curie temperature is another key quantity, since performance at high temperature is of great importance for technological use.

Rare-earth magnets consist of 3*d* transition metals (TM) and rare-earth (RE) elements. Large magnetization is mainly determined from interactions between the TM-3*d* electrons, whereas strong magnetic anisotropy arises from spin-orbit coupling in the RE-4*f* electrons. They couple each other via the RE-5*d* electrons by orbital hybridization and Hund's coupling (see the figure below). The effective Hamiltonian is thus expressed as

$$H_{\mathrm{eff}} = \lambda \mathbf{L} \cdot \mathbf{S} + 2\mathbf{H}_{\mathrm{ex}} \cdot \mathbf{S} + V_{\mathrm{CEF}}$$

Here **L** and **S** denote the orbital and spin operator for the RE-4f electrons, respectively, and V_{CEF} is the crystal electric field. When the spin-orbit coupling is much larger than V_{CEF}, which is usually the case in rare-earth magnets, single-ion anisotropy originating from V_{CEF} gives a measure of the strength of magnetic anisotropy. Material dependence and temperature effects on magnetic properties are major issues.

In my presentation, I will show results of first-principles calculation for typical rare-earth magnets, and discuss their magnetic properties.