## Must for candidates of permanent magnet materials

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The basic strategy of designing a new permanent magnet material is to attain a large saturation magnetization  $M_{\rm S}$ , a high Curie temperature  $T_{\rm C}$ , and a strong magnetic anisotropy in a single crystal. The question is then if there are some limits to these quantities and, if it is, what are the values and what determine them. The answer to the first question is "yes". Concerning the second and third questions, obviously the magnetization cannot exceed the local atomic magnetization, which is limited to  $\sim 5 \mu_B$  (transition metals) or  $\sim 10 \mu_B$  (rare earths) per atomic volume; our experience tells that the possible maximum  $M_{\rm S}$  probably is not larger than 2.5 T that is attained for Fe<sub>70</sub>Co<sub>30</sub> alloy (owing to subtle balance between the magnetic moment and volume, see Fig. 1). T<sub>C</sub> do not exceed both the intra-atomic coulombic interaction and bandwidth, which could be ~5 eV, being much higher than the melting temperature. Therefore,  $T_{\rm C}$  ~1500 K might be a good estimate of the limit (enough for practical purposes). The magnetic anisotropy originates from the combination of a crystal structure and the spin-orbit coupling. The crystal structure gives rise to a crystal field as well as anisotropy in kinetic energy. The effects could again reach as large as the bandwidth. On the other hand, the strength of the spin-orbit coupling do not exceed  $\sim 0.1 \text{ eV}$  even for rare earths. Yet another limitation comes from the exchange coupling: if the atoms that possess a large spin-orbit coupling are different from those carrying magnetic moments, the exchange coupling between those two types of atoms limits the strength of magnetic anisotropy. Eventually, the magnetic anisotropy is limited by the spin-orbit coupling in the case of transition metals and the crystal field (including kinetic part) in the case of rare earths. From such arguments, it may be realistic to define the following figures for an ultimate permanent magnet material:  $M_{\rm S} \sim 2.5$ T,  $T_{\rm C} \sim 1500$  K, and  $K_1 \sim 50$  MJ/m<sup>3</sup>

In order to realize the above figures to some extent, the following considerations might be helpful: First, the material should be definitely metallic so that the ferromagnetism can be the most stable magnetic structure. For this it is necessary that the main player, Fe, be in a metallic environment. The adding some amount of Co would help to increase  $M_{\rm S}$  and  $T_{\rm C}$ . Moreover, for the ferromagnetic state to be stable, each Fe should take approximately a six coordinate bcc-like structure. In such a situation, high  $T_{\rm C}$  is also guaranteed. Concerning the magnetic anisotropy, it is impossible to attain enough anisotropy with using only transition metal elements: though realizing a highly tetragonal lattice might be possible, the spin orbit coupling will not be strong enough to fix the magnetic moment to the lattice. Then the maximum of  $K_1$  would be ~  $5\text{MJ/m}^3$ . To obtain  $K_1$  one order of magnitude bigger than that definitely needs the existence of rare earths in the system, as is supported by experiences. For example, at law temperature, the magnetic anisotropy is still owing to the rare earth although the number of rare earth atoms in the unit cell is much smaller than that of Fe atoms.

Further detailed discussion about the must for candidates of permanent magnet materials will be discussed on the basis of first-principles calculation of magnetic and electronic properties of magnetic materials.



Fig. 1 the magnetic moment (left) and the magnetization  $M_s$  as functions of the lattice constant and fictitious nuclear number. The arrows indicate the lattice constant corresponding the minimum of the total energy of the system.