

Magnetic properties of rare earth mixed crystal magnet materials

H. Akai

*Institute for Solid State Physics, University of Tokyo
Kashiwa-no-ha, Kashiwa, Chiba 277-8581*

The purpose of the present study is to develop a system that can generate permanent magnet materials databases in the multi-dimensional composition spaces by using first-principles electronic structure calculation. Given a structure and a set of components, e.g., $\text{Sm}(\text{Fe}_{1-x}\text{Co}_x)_{12}(\text{N}_{1-y}\text{S}_y)$, we typically need calculations for 100~1000 different systems. Since these systems are compositionally disordered, usual band structure calculation is not suitable for realistic simulations. An efficient way to handle this problem is to use the KKR-CPA method, which can take a configurational average of such disordered systems rather accurately. Unfortunately, the full-potential scheme is not implemented in the present version of KKR-CPA used now[1] (full-potential KKR-CPA codes exist but they do not suit the present purpose because of their heavy computational demands). On the other hand, the pseudo-potential codes can calculate the ordered system quite efficiently although their accuracy has to be checked from time to time through comparisons with the results obtained by other more reliable method such as full-potential KKR and WIEN2k. Considering the above, one of the practical ways to take is to combine KKR-CPA and pseudo-potential codes: use pseudo-potential codes for the end points (i.e., ordered alloys) of composition space and use KKR-CPA to interpolate all the remaining region of the space. A computational system “HOFMAN” constructed under such a strategy is now running.

An example of the usage of HOFMAN system is seen in Fig. 1, where a new alloy system $\text{Sm}(\text{Fe}_{1-x}\text{Co}_x)_{12}(\text{N}_{1-y}\text{S}_y)$ is examined.

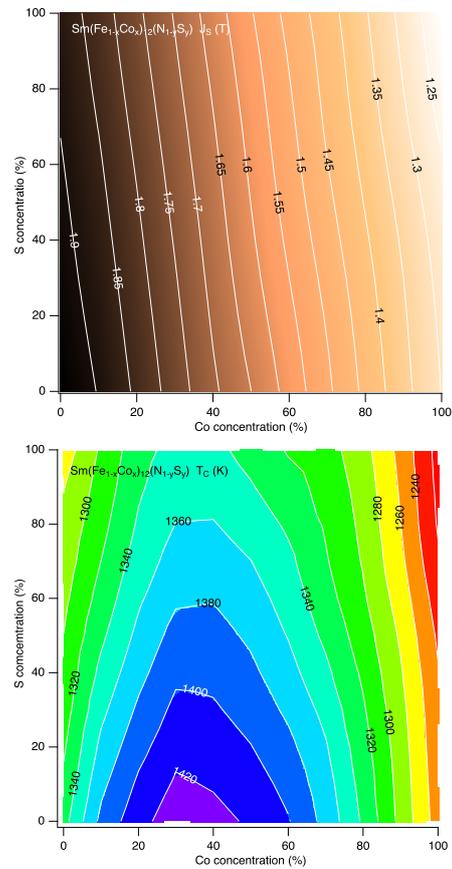


Figure 1: Magnetization (T) (top) and T_C (K) (bottom) of $\text{Sm}(\text{Fe}_{1-x}\text{Co}_x)_{12}(\text{N}_{1-y}\text{S}_y)$.

References

- [1] H. Akai, AkaiKKR, <http://kkp.iissp.u-tokyo.ac.jp/> (2002).