Systematics of Curie temperature in rare earth permanent magnet materials

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Curie temperatures T_C's of permanent-magnet materials R_2(Fe,Co)$_{14}$B, R_2(Fe,Co)$_{17}$, and RFe$_{11.5}$Ti$_{0.5}$ (R = La, Ce,..., Lu, Y), are calculated within the mean field approximation using the exchange coupling constants J_{ij}'s that are obtained by first-principles KKR–Green's function method[1]. While the agreement between the calculations and experiments is rather well for the Co-based systems, there arise some discrepancies in the case of Fe-bases systems. Despite these discrepancies, however, the systematic changes seen in T_C as the rare earth element R changes across the lantanoid are fairly well reproduced by the calculation. In the case of R_2Fe$_{14}$B, the discrepancies can be largely diminished by using J_{ij}'s that are calculated for local-moment disordered states (LMD), which is considered to correspond to the paramagnetic state above T_C, as is shown in Fig.1 and 2. However, this is not the case in general: the discrepancies seen in R_2Fe$_{17}$ (FIg. 3), cannot be remedied. From the analyses of calculated and experimental data, it is concluded that data assimilations are possible and necessary to make reasonable predictions of T_C for rare earth permanent-magnet materials, in particular, the Fe-based ones.

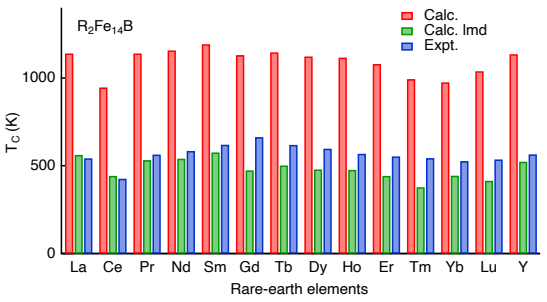

Figure 1: Calculated T_C of R_2Fe$_{14}$B compared with experiments.

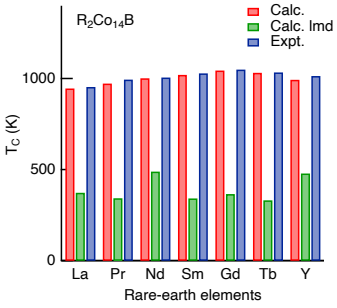

Figure 2: Calculated T_C of R_2Co$_{14}$B compared with experiments.

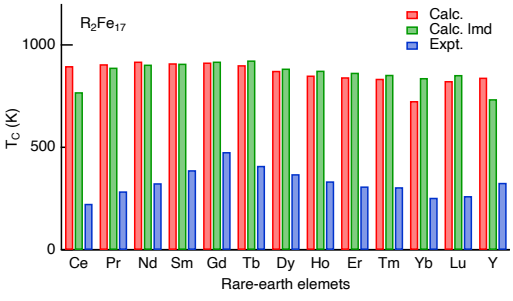

Figure 3: Calculated T_C of R_2Fe$_{17}$ compared with experiments.

References

[1] H. Akai, AkaiKKR, `http://kkr.issp.u-tokyo.ac.jp/` (2002).