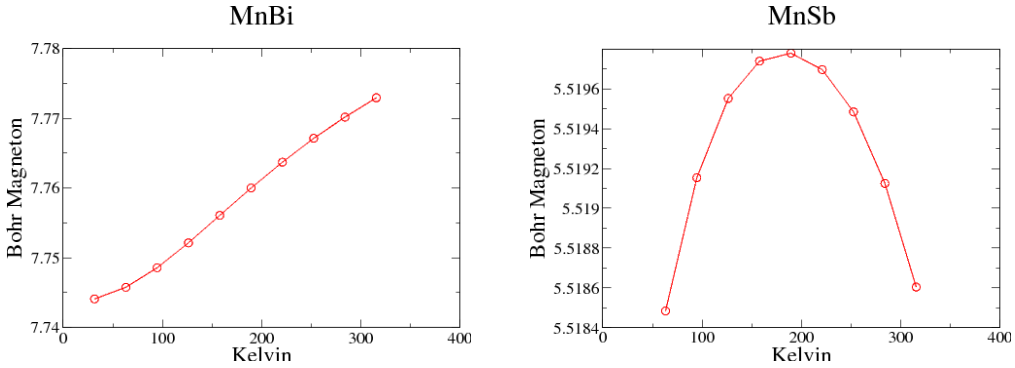
Thermo-magnetic Properties of Rare-earth Replacement Magnetic Materials: MnBi and MnSb

Soo Kyung Kim, Dongsheng Li, Moe Khaleel and Kim F. Ferris*
Pacific Northwest National Laboratory
Fundamental and Computational Materials Sciences Directorate
Richland, WA 99352

Hamid Garmestani
Georgia Institute of Technology
School of Materials Science and Engineering
Atlanta, GA 30332

MnBi and MnSb are both ferromagnetic metals with strong magnet energy products giving rise to their candidacies as replacement materials for the rare earth compounds. Both materials have NiAs structure type structures at room temperature, with small differences in their Curie temperatures (628 and 585 K respectively). However, MnBi has gained much attention due to unique positive temperature coefficient for coercivity and large uniaxial magnetic anisotropy. Several proposed mechanisms have been discussed as the origin of this phenomenon. One, a structural phase transition occurring at higher temperatures may affect MnSb, compared to the relatively stable MnBi form. Also, thermal excitation involving additional electronic states may be differentially affecting MnSb. Both would affect the exchange coupling leading the deviation of magnetic moment from the easy direction, c-axis.

To investigate those factors controlling the positive temperature dependence, we have performed a series of first principles electronic structure calculation on the thermo magnetic properties of MnBi and MnSb. The total magnetization in the easy direction of magnetic moment has been calculated as a function of temperature in the range from 30K to 315K for these two compounds. Temperature effects were examined with fixed electronic temperature using cold smearing. Calculations have been performed for the hexagonal NiAs-type structure which is considered as the stable structure at room temperature, and the MnP structure experimentally observed for MnAs at low temperatures (T< 398K). Preliminary results (Figure below) show the monotonic positive thermo-magnetic coefficient in MnBi in contrast to the convex pattern of thermo magnetic coefficient in MnSb compound. Factors affecting the exchange coupling in these compounds are investigated to guide materials design of new rare earth replacement magnetic materials.



* Tel.: +1-509 375 3754; Fax: +1-5093752522. Email: kim.ferris@pnnl.gov . This work was supported by the U.S. Department of Energy/Office of Science under contract DE-AC06-76RLO 1830.