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Tight binding model for magneto-crystalline anisotropy in MnBi

K. V. Shanavas
Materials Science and Technology Division, Oak Ridge National Laboratory,
Oak Ridge, Tennessee 37831-6056, USA.
Email: kavungalvees@ornl.gov

Abstract With the help of density functional theory based first-principles calculations and a tight-binding model Hamiltonian we studied the origin of magnetic properties in the ferromagnet MnBi. The model Hamiltonian show that direct electron hopping within the nearest and next nearest Bi-*p* orbitals are responsible for the large band dispersions. The Mn-*d* bands are fairly narrow with band widths < 2 eV. A Stoner model with spin-orbit coupling leads to the observed negative MAE with this Hamiltonian.

Keywords: First-principles, tight-binding, model Hamiltonian, magnetism, magnetic anisotropy.

Background

The future of clean energy technologies depend critically on developing new cheaper permanent magnet materials with fewer rare-earth elements.[1] To be a hard magnet, a material should possess large axial magnetocrystalline anisotropy energy (MAE) in addition to large Curie temperature and saturation moment.[2] MAE originates primarily from spin-orbit coupling, but depends on the details of electronic structure, crystal field and the strength of SOI. MnBi is a good candidate among the transition metal systems because of its large magnetic moment and strong magnetic anisotropy energy (MAE).

In the low-temperature phase, MnBi is a ferromagnetic compound with the NiAs structure. Above 628 K, a first-order paramagnetic transition accompanied by a phase decomposition to $Mn_{1.08}Bi$ takes place.[3] The magnetic phase of MnBi is unusual in that the anisotropy constant (K_u) increases with temperature unlike most magnets. Also, K_u is negative below ~90 K, with all the magnetic moments aligned in the in-plane direction. A spin-reorientation transition takes place at $T_{SR} \approx$ 90 K, when the magnetization changes direction towards *c* axis. Thus, K_u starts at −0.2 MJ/m^3 close to 0 K and reaches 2 MJ/m^3 at room temperature.

Materials and Methods

To understand these features better, we constructed a tight- binding (TB) model Hamiltonian using linear combination of atomic orbitals method. The single electron Hamiltonian has three components:

$$H = H_t + H_M + H_{SO}$$

The first component H_t is the electron band structure term arising from the overlap of atomic orbitals. The periodic nature of the lattice helps us construct the matrix elements $\langle\phi_{\alpha 0}|H_t|\phi_{\beta R}\rangle$ in the reciprocal space by writing the atomic orbitals as a Bloch sum,

$$|\chi_{\alpha k}\rangle = 1/\sqrt{N}\sum_R e^{ik\cdot R}\,|\phi_{\alpha R}\rangle$$

So, that

$$H_t(k) = \varepsilon_{\alpha\delta_{\alpha\beta}} + \sum_{\langle R\rangle} e^{ik\cdot R} H_t(R)$$

which are modeled by two center Slater-Koster parameters, $V_{pp\sigma}, V_{pp\pi}$ etc. The second term H_M is the Stoner magnetic term which can be written as,

$$\langle\phi_{j\beta\sigma'}|H_M|\phi_{i\alpha\sigma}\rangle = \frac{1}{2}\delta_{ij}\delta_{\alpha\beta}I_{i\alpha}\hat{m}\cdot\vec{\tau}_{\sigma\sigma'}$$

where *I* is the Stoner parameter for the orbital, $\hat{m}$ is the magnetic moment, $\vec{\tau}$ are the Pauli matrices and σ is the spin index. The last term H_{SO} is the spin-orbit coupling part.

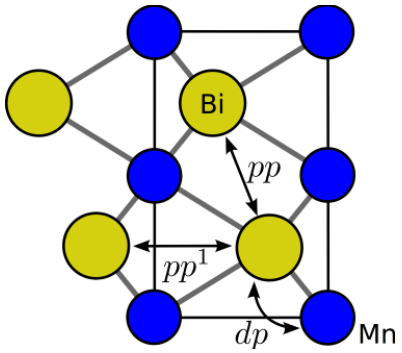

Figure 1. TB hopping parameters. Structure and tight-binding hopping parameters for MnBi crystal viewed along *b* axis.

The basis states included Mn-*d* and Bi-*p* orbitals and the hopping interactions are marked in Fig. 1. Only nearest neighbor *d*–*p* interactions are included for Mn ions. However, owing to their larger size, Bi ions also interact directly via *p*–*p* coupling in addition to *p*-*d* coupling.

Results

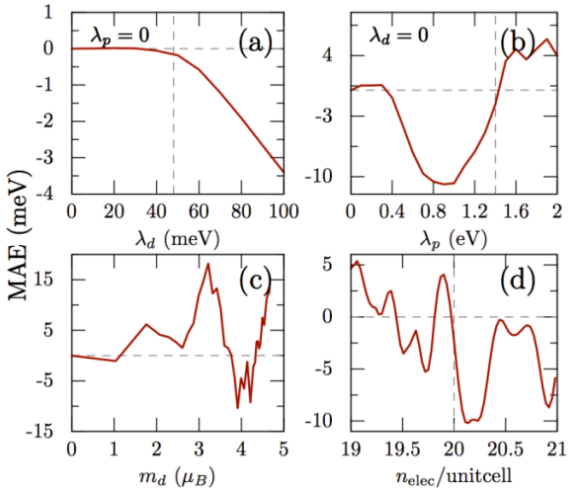

Figure 2. TB results. Magnetic anisotropic energy (MAE) as a function of TB parameters: (a) λ_d is varied with λ_p = 0, (b) λ_p is varied with λ_d = 0, (c) Mn magnetic moment by varying I_d (c) band filling by varying the number of electrons

The model reproduces the magnetic properties of MnBi quite well.[4] With the parameters discussed in Ref 4 and the Mathematica notebook in Ref 5, the tight-binding model is able to reproduce the correct low temperature magnetic ground state. We find a magnetic anisotropy of -2.7 meV, which is overestimated compared to the experimental value of -0.4 meV near 0 K,[6] but has the correct sign. The analytical expressions for the tight-binding part of the Hamiltonian are given in the Mathematica notebook along with typical parameters obtained by fitting with the bands from first principles calculations.

Fig. 2 shows the magnetic anisotropy energy calculated using the full tight-binding Hamiltonian by varying different parameters. The top two panels show the effect of spin-orbit coupling strength on MAE. The SO coupling parameter in Mn atoms are significantly weaker than that of Bi, hence most of the contribution towards MAE comes from Bi atoms. We find that contribution from Bi towards K_1 is -1.5 meV, where as the contribution from Mn is -0.17 meV. Total MAE is -2.7 meV. Interestingly Fig. 1(b) shows that a slightly weaker λ_p would enhance MAE. Infact, a similar material MnSb with smaller SOI has been found to show higher MAE.[7] Fig. 1(d) shows that lower band filling can change the sign of MAE, which agrees qualitatively with previous DFT calculations.[8]

Conclusions

A tight-binding based model Hamiltonian developed to understand the magnetic prpoerties of MnBi is discussed. Direct Mn-Mn interaction is found to be small, but owing to their large size Bi-Bi interaction is found to be important. Parameters of the model are derived from the first-principles band structure calculations.

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