

Influence of Magnetic Material on Tunnel Magnetoresistance and Spin-Transfer Torque in MgO-based Tunnel Junctions

Researchers
C. Mahr, Christian Franz and Dr. Michael Czerner

Principal Investigator
Prof. Dr. Christian Heiliger

Project Term
2015 - 2015

Project Areas
Optics, Quantum Optics and Physics of Atoms, Molecules and Plasmas, Physical and Theoretical Chemistry

Clusters
Skylia Cluster Gießen

Institute
I. Physikalisches Institut

University
Justus Liebig University Giessen

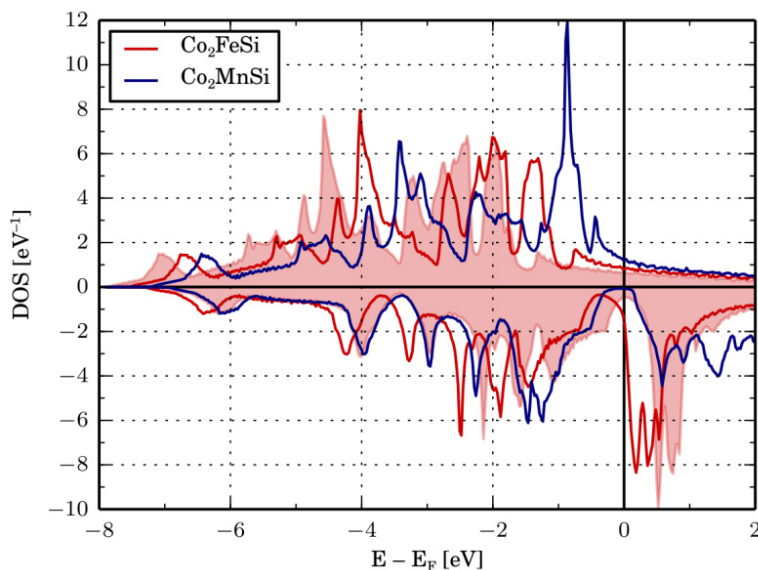


Fig. 1: Density of states for Co₂FeSi (red) and Co₂MnSi (blue) in generalized-gradient approximation (GGA). The latter has a band gap at EF and behaves therefore half-metallic, while the first does not. Filled: FSM calculation.

Introduction

Some Heusler alloys, for example intermetallic compounds of the stoichiometric composition X₂YZ with L2₁ structure,[1] are assumed to be half-metals: one spin direction shows metallic behavior at the Fermi energy EF, while the other channel has an energy gap.[2]

Methods

Thus, they could be employed as spin filters to assemble devices with near infinite (tunnel) magnetoresistance. As they further carry high magnetic moments at the order of 3 to 6μB, [1, 3] they are promising options for the construction of spintransfer torque magnetic random-access memories (STT-MRAMs).

Results

Since our experimental collaborators at Bielefeld university are especially interested in magnetic tunnel junctions (MTJs) containing Co₂FeSi and its inverse Heusler Fe₂CoSi, we

calculated the magnetic moment, band structure, density of states (DOS), and transport properties of bulk Co_2FeSi and, as a reference, Co_2MnSi . These calculations were done using our density-functional theory (DFT) [4] based Korringa-Kohn-Rostocker (KKR) Green's function formalism code.[5] In non-relativistic generalized-gradient approximation (GGA), Co_2FeSi has a magnetic moment which is much lower than the theoretically expected value.[6] In addition, no half-metallic behavior is observed. Although published results vary drastically,[6] our result is still much lower than the average published value. Changes in the exchange-correlation functional produced values as low as $4.94\mu\text{B}$, whilst taking relativistic effects into account proved to be nearly ineffective. Co_2MnSi , in contrast, behaves much better: The magnetic moment in non-relativistic local spin-density approximation (LSDA) is near the theoretically predicted value, and this result may readily be improved by employing a GGA. Further, this Heusler compound displays half-metallic behavior, as the band structure shows a direct band gap at the gamma point for the minority spin polarization, which is reflected in a near zero-valued minimum in the DOS around E_F (Fig.1), and a vanishing transmission rate for the corresponding spin. , 86: 0544

Discussion

We assume that our computational scheme might underestimate the magnetic polarization. To verify this, we implemented a fixed spin-moment (FSM) method, being a slight generalization of.[7] This allows us to perform DFT calculations analogous to (Meinert et al.).[8]

We performed two FSM calculations: The first with the total magnetic moment fixed to the theoretical $6\mu\text{B}$, the second with atomic moments fixed to the experimental values from x-ray magnetic circular dichroism.[8] The effect of both was to shift the minority bands up by $\Delta E/2$ and the majority bands down by the same amount, which lead to corresponding displacements in the DOS. This is to be expected, as the fixation of the magnetic moments is done by shifting the potentials accordingly. Given the case of Co_2FeSi , no band gap opens, and the Heusler thus stays metallic. In conclusion, the possible underestimation of magnetic moments in our computational scheme seems not to be the major issue when trying to predict (half-)metallic behavior.

Outlook

With regard to our results, calculations on $\text{Co}_2\text{Fe}_x\text{Mn}_{1-x}\text{Si}$ might show that the different properties of both alloys may be combined to gain even higher performances.

Reference

- [1] P.J. Webster (1969), Heusler alloys, Contemporary Physics, 10 (6): 559-577. <https://doi.org/10.1080/00107516908204800>
- [2] T. Block, M.J. Carey, B.A. Gurney, and O. Jepsen (2004), Band-structure calculations of the half-metallic ferromagnetism and structural stability of full- and half-Heusler phases, Physical Review B, 70 (20): 205114. <https://doi.org/10.1103/PhysRevB.70.205114> [Titel anhand dieser DOI in Citavi-Projekt übernehmen]
- [3] B. Balke, G.H. Fecher, H.C. Kandpal, C. Felser, K. Kobayashi, E. Ikenaga, J. Kim, and S. Ueda (2006), Properties of the quaternary half-metal-type Heusler alloy $\text{Co}_2\text{Mn}_{1-x}\text{FexSi}$, Physical Review B, 74, 104405. <https://doi.org/10.1103/PhysRevB.74.104405>
- [4] W. Kohn (1999), Nobel Lecture: Electronic structure of matter—wave functions and density functionals, Reviews of Modern Physics, 71 (5), 1253-1266. <https://doi.org/10.1103/RevModPhys.71.1253>
- [5] P. Mavropoulos and N. Papanikolaou (2006), The Korringa-Kohn-Rostoker (KKR) Green Function Method. I. Electronic Structure of Periodic Systems, NIC Series, 31: 131-158, 2006. <https://juser.fz-juelich.de/record/50027/files/FZJ-2014-02214.pdf>
- [6] S. Wurmehl, G.H. Fecher, H.C. Kandpal, V. Ksenofontov, C. Felser, H. Lin, and J. Morais (2005), Geometric, electronic, and magnetic structure of Co_2FeSi : Curie temperature and magnetic moment measurements and calculations, Physical Review B, 72: 184434. <https://doi.org/10.1103/PhysRevB.72.184434>
- [7] K. Schwarz P. and Mohn (1984), Itinerant metamagnetism in YCo_2 , Journal of Physics F: Metal Physics. 14: L129-L134. <https://doi.org/10.1088/0305-4608/14/7/008>
- [8] M. Meinert, J.M. Schmalhorst, M. Glas, G. Reiss, E. Arenholz, T. Böhnert, and K. Nielsch (2012), Insights into the electronic mstructure of Co_2FeSi from x-ray magnetic linear dichroism, Physical Review B, 86: 054420. <https://doi.org/10.1103/PhysRevB.86.054420>

Last Update: 2022-07-14 17:44