Journal of Magnetism and Magnetic Materials 322 (2010) 1082–1084

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Does a Heisenberg Hamiltonian describe magnetic interactions in a MnSi film properly?

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ARTICLE INFO

Available online 11 March 2009

Keywords:
Exchange parameter

ABSTRACT

We report theoretical studies of magnetic excitations in an ultra-thin MnSi film on Si(0 0 1) substrate. Both transversal and longitudinal fluctuations of the magnetic moments are discussed. We show that the values of the Heisenberg exchange parameters depend on the assumed distance of the short range magnetic order and on the values of the atomic moments. The limitations of the mapping of the system on a Heisenberg model are studied.

1. Introduction

The epitaxial growth of MnSi on Si(0 0 1) has been studied in the context of spintronics aiming to realize spin injection through a metal-semiconductor interface. Two important requirements on the magnetic materials for the spintronic applications are: (i) a high spin polarization of the electronic states at the Fermi level, (ii) a Curie temperature substantially exceeding room temperature. Theoretical investigation [1–3] predicted a ferromagnetic ground state for a thin MnSi film with B2-type crystal structure grown on Si(1 0 0). It was found that the MnSi B2-films have a high degree of spin polarization at the Fermi level between 30% and 50%, depending on film thickness [2,3].

To study the thermal stability of the ferromagnetic state we mapped the system on a Heisenberg Hamiltonian with first and second nearest neighbor interactions. The Curie temperature was estimated within the mean-field and within the random-phase approximation. The calculated values exceed 200 K for a one monolayer (ML) MnSi film and 300 K for a two ML MnSi film [4].

The purpose of the given paper is to study the limitations of the mapping of the magnetic MnSi interactions on a Heisenberg model. Two types of the limitations exist. First, in the models where only the directions of the atomic moments are considered as degrees of freedom (transversal fluctuation) higher order spin interactions are neglected. Second, in itinerant electron systems the atomic moments can fluctuate not only in direction but also in magnitude (longitudinal fluctuations).

2. Calculational details

The mapping on a model Hamiltonian is a usual approach to study the thermodynamics of itinerant electron systems. For a multi-sublattice crystalline system the Heisenberg Hamiltonian can be written in the form

$$H_{\mathrm{Heis}} = -\sum_{i,j}\sum_{\mathbf{R},\mathbf{R}'} J^{i,j}_{\mathbf{R},\mathbf{R}'}\mathbf{M}^{i}_{\mathbf{R}}\cdot\mathbf{M}^{j}_{\mathbf{R}'}, \tag{1}$$

where the indices i,j indicate different sublattices and $\mathbf{R}$ and $\mathbf{R}'$ are the lattice vectors specifying the atoms within sublattices, $\mathbf{M}_{\mathbf{R}}$ is the vector pointing in the direction of the magnetic moment at site, $\mathbf{R}$.

In the case of MnSi/Si(0 0 1) there are two inequivalent Mn sublattices in the surface unit cell. We will refer to the sublattices as Mn_1 and Mn_2. The directions of the magnetic moments are defined by the unit vectors $(\sin\theta_i\cos\phi_i, \sin\theta_i\sin\phi_i, \cos\theta_i)$ where θ_i and ϕ_i are polar and azimuthal angles.

We consider the magnetic configurations obtained by rotations of the moments on the Mn sublattices with respect to the global z axis by the same angle θ. Within each of the sublattices the atomic moments remain parallel. The azimuthal angles of the two sublattices are different: $\phi_1 = 0$ and $\phi_2 = 180$. The Heisenberg model (Eq. (1)) gives in this case a cosine-type dependence of the energy of the magnetic configurations on the angle 2θ between the moments of the sublattices

$$E_{tr}(\theta) = A(1-\cos 2\theta). \tag{2}$$

Here the energy refers to the ferromagnetic state and A is constant. Therefore the deviation of the calculated energy from the cosine-type dependence can be used as a measure to test the validity of the Heisenberg model.

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doi:10.1016/j.jmmm.2009.03.007

Our calculations are performed within the framework of the density functional theory (DFT) using the augmented spherical wave (ASW) method [6,7]. The local spin density approximation (LSDA) to the exchange-correlation potential is employed. To study the longitudinal atomic fluctuations we use a constrained minimization of the total energy functional. The desired value of the atomic moment m is stabilized by an effective constraining magnetic field that depends on m and is determined self-consistently.

3. Results and discussion

In Ref. [4] we estimated the Curie temperature of a one ML MnSi film using a Heisenberg model with interatomic exchange parameters determined from energy differences of several collinear magnetic configurations [4].

Here we consider noncollinear magnetic configurations with different angles between the magnetic moments. The angle $\theta = 90^\circ$ corresponds to the antiferromagnetic configuration. The energy of the antiferromagnetic state is in good agreement with our previous calculation of collinear spin configurations using the FP-LAPW method [4].

To verify how well the calculated data are described by the Heisenberg model we compare the calculated band energies with the Heisenberg-type dependence (Eq. (2)). The parameter $A = 0.088$ eV is chosen to scale the Heisenberg curve according to the calculated θ-dependence (Fig. 1). The comparison shows a considerable deviation of calculated energies from simple cosine-like behavior. The deviations from the cosine function are rather symmetric with respect to angle $\theta = 45^\circ$ (c.f. dotted curve in Fig. 1).

The ratio of the Heisenberg energy (Eq. (2)) to $1 - \cos 2\theta$ is independent of theta. However, a similar ratio for the calculated curve shows strong θ-dependence (Fig. 2) varying from 6.8 meV at small θ to 11.0 meV for $\theta = 90^\circ$. The strong θ-dependence of J indicates the limited validity of the Heisenberg model taking into account transversal fluctuations. A way out of this limitation is to include higher-order interactions such as, biquadratic and three-spin interactions. In a qualitative manner the deviation from the Heisenberg model can be treated as a θ-dependence of the exchange parameters. Then the choice of the proper exchange parameters depends on the characteristic angles between atomic moments. The assumption of a very strong short range magnetic order (SRMO) corresponds to low-θ values of the exchange interaction. On the other hand, if the SRMO is negligible the average angle between different moments is 90° and values of the exchange interaction should be taken from the large-θ calculations. The mean-field estimation of the Curie temperature assuming nearest-neighbor exchange interactions and using low-θ values of the parameters gives 230 K whereas the large-θ parameter results in 380 K. Unfortunately at present a direct experimental determination of the strength of SRMO does not exist. An optimal choice of the strength of the SRMO needs further studies.

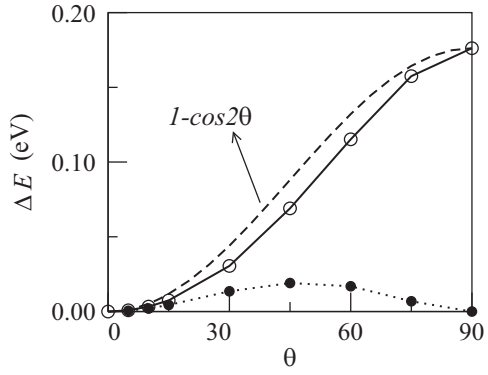

Fig. 1. The total energy as a function of angle θ of the magnetic moments of the Mn sublattices in MnSi/Si(0 0 1) (solid line). The dashed curve represents a Heisenberg-type dependence. The dotted curve gives the difference between the calculated and Heisenberg-type dependencies.

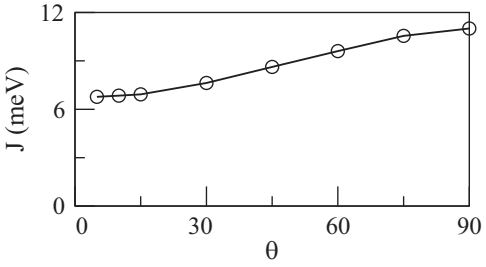

Fig. 2. The exchange interaction as function of angle θ.

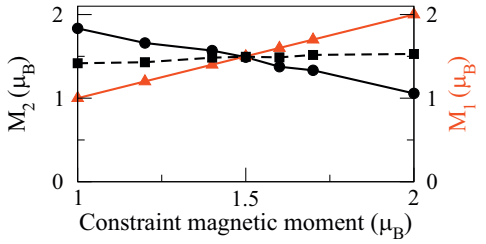

Fig. 3. (Color online) The change of the sublattice (solid lines with circles and triangles) and total (dashed line) magnetic moments as a function of the value of the constrained magnetic moment of the first sublattice.

Besides the transversal fluctuations the longitudinal fluctuation of the atomic moments contribute to the thermodynamic properties. The variation of the magnitude of the atomic moments is neglected in the Heisenberg model. To study longitudinal fluctuations we consider the ferromagnetic ground state and impose a constraining field on the atoms of one of the Mn sublattices. The calculations show that the effect of the constraining field is not restricted to the sublattice where it is applied. Because of the interatomic hybridization also the moments of the atoms of the second sublattice change.

Fig. 3 shows the variation of the magnetic moments of the Mn sublattices as well as the total magnetic moment per unit cell as a function of constraint imposed on the Mn_1 atom. Rather unexpectedly the increase of the magnetic moment of the Mn_1 atom causes the decrease of the moment of the Mn_2 atoms. The changes of the moments of two Mn atoms almost compensate each other. Therefore the total moment of the unit cell is nearly constant. A similar type of relation was recently obtained between induced and inducing magnetic moments in half-metallic compounds NiMnSb. [8].

In Fig. 4, we show the total energy as a function of the value of the Mn_1 moment. The energy as a function of the Mn_1 moment has a shape of an asymmetric parabola-like function with a minimum at the ground-state value of the moment. A fit of the energy curve around the minimum with the function $y = a(x - m_0)^2$ gives the coefficient $a = 82\,\text{meV}/\mu_B^2$. The contribution of the longitudinal fluctuations at a given temperature depends on the interval of the values of the magnetic moment corresponding to the energy variation of the order of k_BT. The flatter the curve, the smaller is a and the larger is the contribution of the longitudinal fluctuations.

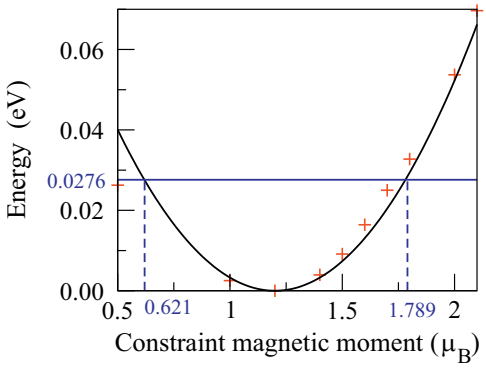

Fig. 4. (Color online) The total energy as a function of constrained magnetic moment of the first Mn sublattice. The blue solid line refers to the mean-field energy of transversal fluctuations at $\theta = 15^{\circ}$.

The contribution of the longitudinal fluctuations is small if the characteristic energies of the transversal fluctuations described by the Heisenberg Hamiltonian are much smaller than the characteristic energies of the deviation of the atomic moments from the values at the minimum of the total energy. To estimate the influence of the longitudinal fluctuations, we compare the value of the Heisenberg mean-field energy $E_M = nJ$ where n is the number of the nearest neighbors and J the nearest-neighbor exchange interaction. Using $J = 6.9$ meV corresponding to $\theta = 15^{\circ}$ in Fig. 2 we get $E_M = 27.6$ meV. Taking this energy as a maximal energy of the longitudinal fluctuation of the Mn_1 moment the fluctuation interval is $0.621 < M < 1.785$ (see Fig. 4 blue lines). Therefore the contribution of longitudinal spin fluctuations to the thermodynamics of the MnSi films is expected to be considerable and should be taken into the account.

On the basis of the considerations suggested above the energy of an arbitrary magnetic configuration with respect to the ground-state energy contains the contribution coming from the change of the relative directions of the atomic moments and the contribution caused by the change of the values of the atomic moments. The first contribution is determined by the interatomic exchange parameters and the second by the longitudinal stiffness of the moments. However, in general, these contributions are not independent of each other. In Fig. 5 we show the values of the

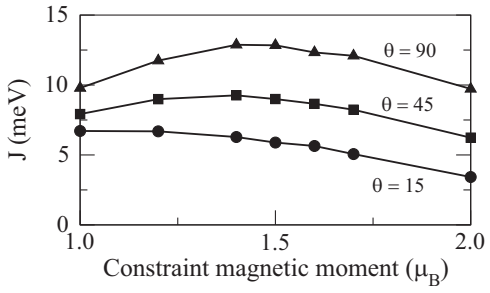

Fig. 5. The exchange coupling as a function of the constrained magnetic moment of the Mn_1. The dependencies are present for three values of the angle θ of the moments of the Mn sublattices.

interatomic exchange interactions as a function of the value of the Mn_1 moment calculated for different values of the angle θ between the moments of two Mn sublattices. We see that the dependence on the value of the moment is considerable and is different for different θ.

A standard Heisenberg model is not able to describe the thermodynamics and the magnetic interactions in a MnSi film correctly. Higher order magnetic interaction have to be considered adequately.

Acknowledgments

We would like to thank Matthias Scheffler and Peter Kratzer for initiating the project and valuable discussions.

References

[1] H. Wu, M. Hortamani, P. Kratzer, M. Scheffler, Phys. Rev. Lett. 92 (2004) 237202.
[2] M. Hortamani, H. Wu, P. Kratzer, M. Scheffler, Phys. Rev. B 74 (2006) 205305.
[3] M. Hortamani, Theory of adsorption, diffusion and spin polarization of Mn on Si(0 0 1) and Si(1 1 1) substrates, Ph.D. Thesis, Freie universität, Berlin, 2006.
[4] M. Hortamani, L.M. Sandratskii, P. Kratzer, I. Mertig, M. Scheffler, Phys. Rev. B 78 (2008) 104402.
[6] A.R. Williams, J. Kübler, C.D. Gelatt, Phys. Rev. B 19 (1979) 6094.
[7] L.M. Sandratskii, Adv. Phys. 47 (1998) 91.
[8] L.M. Sandratskii, Phys. Rev. B 78 (2008) 094425.