Exchange interactions and Curie temperatures of 3D- and 2D-ferromagnets *)

J. Kudrnovský, V. Drchal

Institute of Physics, Acad. Sci. CR,
Na Slovance 2, CZ-182 21 Praha 8, Czech Republic

I. Turek,**)

Institute of Physics of Materials, Acad. Sci. CR,
Žižkova 22, CZ-616 62 Brno, Czech Republic

M. Pajda, P. Bruno

Max-Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany

Received 8 October 2001

Effective exchange interactions in bulk ferromagnets as well as in magnetic overlayers on Cu(001) covered by a Cu-cap layer of varying thickness were determined from first principles by mapping of corresponding total energies onto the effective Heisenberg model in the framework of the adiabatic approximation and magnetic force theorem. The effective Heisenberg model is then used to determine spin-wave stiffness constants and Curie temperatures evaluated in the framework of the random-phase approximation. Calculations are in a fair agreement with available experimental data for bulk ferromagnets and reproduce an oscillatory Curie temperature of magnetic overlayers as a function of Cu-cap thickness in a qualitative agreement with recent experiments.

PACS: 71.15.-m, 75.10.-b
Key words: Curie temperature, spin-wave stiffness constant, first-principles calculations, bulk ferromagnet and magnetic multilayers

1 Introduction

In spite of a considerable effort in last decades a first-principles calculation of thermodynamic properties of solids remains a very serious challenge to the theory. For example, the evaluation of the Curie temperature of bulk ferromagnets and, in particular, of two-dimensional systems has to rely upon some approximation schemes. A simple and yet accurate approach consists in a mapping of the complicated itinerant electron system onto an effective Heisenberg model (EHM), $H = -\sum_{i \neq j} J_{ij}\ \mathbf{e}_i \cdot \mathbf{e}_j$, where $\mathbf{e}_i$ and $\mathbf{e}_j$ are the unit vectors of the magnetic moments at sites i and j, and the effective exchange interactions (EEIs) J_{ij} between any pair of magnetic moments are determined from first-principles. This

*) Presented at 11th Czech and Slovak Conference on Magnetism, Košice, 20–23 August 2001
**) Also at *Depatment of Electronic Structures, Charles University, Prague, Czech Republic*

approach proposed by Liechtenstein [1] for bulk systems can be also generalized to low-dimensional systems [2]. The thermodynamic properties of the ferromagnet including determination of the Curie temperature can be then calculated from the EHM by using statistical mechanical methods. The success of this two-step approach relies upon the fact that it provides an almost exact description of low-lying magnetic excitations (spin-waves) which give the most important contribution to the Curie temperature. We have recently applied this approach to bulk bcc-Fe, fcc-Co, and fcc-Ni [3] as well as to Fe/Cu(001) and Co/Cu(001) overlayers covered by a Cu-cap layer [2] and in this paper we summarize our results.

2 Formalism

The electronic structure of the system is determined in the framework of the first principles scalar-relativistic tight-binding linear muffin-tin orbital method (TB-LMTO) generalized to surfaces [4]. The expression for the EEIs between two sites i and j in the system which carry magnetic moments, namely (i) bulk ferromagnet and (ii) magnetic overlayers on the non-magnetic substrate covered by a Cu cap-layer of varying thickness, reads as

$$J_{ij}^{(n)} = \frac{1}{4\pi}\,\mathrm{Im}\int_C \mathrm{tr}_L\,\left\{\delta_i^{(n)}(z)\,g_{ij}^{(n)\uparrow}(z)\,\delta_j^{(n)}(z)\,g_{ji}^{(n)\downarrow}(z)\right\}\,\mathrm{d}z\,. \tag{1}$$

Here tr_L denotes the trace over the angular momentum $L = (\ell m)$, $\delta_i^{(n)}(z) = P_i^{(n)\uparrow}(z) - P_i^{(n)\downarrow}(z)$ where $P_i^{(n)\sigma}(z)$ are L-diagonal matrices of potential functions of the TB-LMTO method ($\sigma = \uparrow, \downarrow$), energy integration is performed in the upper half of the complex energy plane over a contour C starting below the bottom of the valence band and ending at the Fermi energy, and $g_{ij}^{(n)\sigma}(z)$ are the site off-diagonal blocks of the system Green function corresponding to a given geometry. The superscript refers to the number n of cap-layers (the limit $n = 0$ corresponds to uncovered overlayer case) and it is missing in the bulk case.

The expressions for the spin-wave stiffness constant $D^{(n)}$ and the Curie temperature $T_{\mathrm{c}}^{(n)}$ in the random-phase approximation (RPA) represent a generalization of bulk formalism [1, 3]to the case of magnetic monolayers covered by varying thickness of the non-magnetic cap:

$$\begin{aligned} D^{(n)} &= C\,\frac{\mu_{\mathrm{B}}}{M^{(n)}}\sum_{i\neq 0} J_{0i}^{(n)} R_{0i}^2\,, \quad \frac{1}{k_{\mathrm{B}}T_c^{(n)}} = \frac{6\mu_{\mathrm{B}}}{M^{(n)}}\,\frac{1}{N}\sum_{\mathbf{q}}\,\frac{1}{E^{(n)}(\mathbf{q})}\,, \\ E^{(n)}(\mathbf{q}) &= \Delta^{(n)} + \frac{4\mu_{\mathrm{B}}}{M^{(n)}}\sum_{i\neq 0} J_{0i}^{(n)}\,\left[1 - \exp(\mathrm{i}\mathbf{q}\cdot\mathbf{R}_i)\right]\,. \end{aligned} \tag{2}$$

Here, the $\mathbf{q}$-sum extends over the corresponding Brillouin zone (BZ), N is the number of sites in the BZ, μ_{B} is the Bohr magneton, $R_{0i} = |\mathbf{R_0} - \mathbf{R_i}|$ is the interatomic distance, $M^{(n)}$ is the (layer) magnetic moment per atom, the constant

$C = 1$ and $C = 2/3$ for the overlayer and the bulk ferromagnet, respectively, and $E^{(n)}(\mathbf{q})$ denotes the spin-wave spectrum. A vanishing $T_c^{(n)}$ is obtained in the non-relativistic case in an agreement with the Mermin–Wagner theorem [5] and small relativistic effects, namely the anisotropy energy $\Delta^{(n)}$, have to be considered in order to obtain a non-vanishing value of $T_c^{(n)}$. The anisotropy energy Δ is taken here as an adjustable parameter although it could be determined from first principles. The RPA Curie temperature has only a weak logarithmic dependence upon Δ [2] and it is thus sufficient to know the order of magnitude of Δ. The sum for the evaluation of the spin-wave stiffness constant is non-convergent due to the RKKY character of magnetic interactions in metallic systems and to overcome this difficulty we have calculated it by a regularization procedure [3].

3 Results

The results for bulk bcc-Fe and fcc-Co ferromagnets are presented in Table 1. We obtained a good agreement with available experimental results for both the spin-wave stiffnes and the Curie temperature. It should be noted that conventional mean-field approximation [1, 3] overestimates the Curie temperature giving 1414 K and 1645 K for bcc Fe and fcc Co, respectively.

Table 1. Calculated spin-wave stiffness constants ($D_{\rm th}$) and Curie temperatures ($T_{\rm th}$) and their comparison with experimental values $D_{\rm ex}$ and $T_{\rm ex}$. Two different values for $D_{\rm ex}$ correspond to different experiments.

Metal	$D_{\rm th}$(meV·Å^2)	$D_{\rm ex}$(meV·Å^2)	$T_{\rm th}$(K)	$T_{\rm ex}$(K)
bcc Fe	250	280, 330	950	1044
fcc Co	663	510, 580	1311	1388

Calculated spin-wave spectrum for bcc Fe compares also very well with experiment [3]. The results for fcc-Ni, both the spin-wave stiffness constant and the Curie temperature, does not agree with experiment so well [3] probably because of the neglect of Stoner excitations in the present paper which may be important for nickel (this violates the assumption on the validity of the adiabatic approximation).

The results illustrating the oscillatory dependence of the Curie temperature as a function of the Cu cap-layer thickness are presented in Fig. 1 for the case of Fe-monolayer on Cu(001). The anisotropy energy used in calculations was $\Delta^{(n)} \approx 0.15$ mRy. The oscillatory behavior is in a qualitative agreement with recent experiments [6, 7] and the theory also predicts similar oscillations of spin-wave stiffness constants. These oscilations can be traced down to the oscillatory behavior of the EEIs which in turn is due to the formation of quantum-well states in the cap layer: the barrier is formed on one side by the vacuum and on the other side by the effective barrier due to very different electronic structure of the minority Fe-bands as compared to Cu-bands of the cap-layer. The position of these quantum states

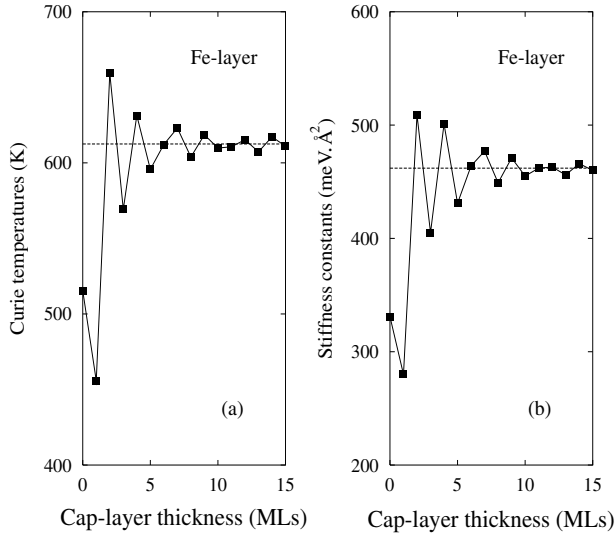

Fig. 1. The Curie temperatures (a) and the spin-wave stiffness constants (b) for Fe-monolayer on fcc-Cu(001) as a function of the cap-layer thickness. The dashed lines represent the embedded layer limit (infinite cap thickness) while the limit of zero cap thickness corresponds to the uncovered overlayer case.

varies with the cap thickness leading thus to corresponding changes in the electronic structure and in the EEIs.

J. K., V. D., and I. T. acknowledge the financial support provided by the Grant Agency of the Czech Republic (No. 202/00/0122), the Acad. Sci. CR (No. A1010829), and the Czech Ministry of Education, Youth and Sports (OC P3.40, OC P3.70, and ME 383).

References

[1] A.I. Liechtenstein, M.I. Katsnelson, V.P. Antropov, and V.A. Gubanov: J. Magn. Magn. Mater. **67** (1987) 65.

[2] M. Pajda, J. Kudrnovský, V. Drchal, I. Turek, and P. Bruno: Phys. Rev. Lett. **85** (2000) 5424.

[3] M. Pajda, J. Kudrnovský, V. Drchal, I. Turek, and P. Bruno: arXiv: cond-mat/0007441.

[4] I. Turek, V. Drchal, J. Kudrnovský, M. Šob, and P. Weinberger: *Electronic Structure of Disordered Alloys, Surfaces and Interfaces*. Kluwer, Boston, 1997.

[5] N.D. Mermin and H. Wagner: Phys. Rev. Lett. **17** (1966) 1133.

[6] R. Vollmer, S. van Dijken, M. Schleberger, and J. Kirschner: Phys. Rev. B **61** (2000) 1303.

[7] A. Ney, F. Wilhelm, M. Farle, P. Poulopoulos, P. Srivastava, and K. Baberschke: Phys. Rev. B **59** (1999) R3928.