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# Ab initio calculation of Heisenberg parameters and Curie temperatures in thin magnetic films

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**Abstract**

We present first principles calculations of the Heisenberg exchange parameters, $J_{ij}$ in thin Co and Ni films on a Cu (0 0 1) substrate. Two methods are compared, relying either on a disordered local moment description of the paramagnetic state or on the magnetically ordered ground state. Ferromagnetic nearest-neighbor and next-nearest-neighbor interactions are found to play a dominating role throughout. Furthermore, $J_{ij}$s display significant dependence on the layer positions, having a typical maximum for layers near the surface of the film as well as at the interface with the substrate. The Curie temperatures calculated within a simple statistical mean-field approach follow qualitatively well the trends against the film thickness observed in the experiments. 

*Keywords:* Magnetic films; Surface magnetism; Exchange interactions; Classical spin models; Curie temperature

## 1. Introduction

Various types of magnetic phase transitions in thin films have attracted much experimental and theoretical effort during the recent decade. One particularly important phenomenon is the dependence of the Curie temperature with respect to several parameters, such as the film thickness, the geometrical structure or the composition of the film. While methods with different sophistication of the statistical mechanics based on Ising or Heisenberg type of Hamiltonians were able to elucidate, e.g., the general features of $T_C$ as a function of the film thickness [1,2], the need for obtaining realistic, material specific parameters which enter these models is obvious.

For layered systems the Heisenberg-model can be written as

$$H = \frac{1}{2}\sum_{pq}\sum_{ij} J_{pi,qj}\, \boldsymbol{S}_{pi}\, \boldsymbol{S}_{qj}, \tag{1}$$

where $\boldsymbol{S}_{pi}$ denotes a classical vector-spin of unit length located at the $i$th site of layer $p$, $J_{pi,qj}$ is the exchange interaction between two particular sites ($pi$) and ($qj$) ($J_{pi,pi} = 0$) and the factor $\frac{1}{2}$ corrects for double-counting. In the present contribution we apply two techniques to calculate exchange interactions in FCC Co and Ni films on Cu(0 0 1), namely, the effective pair interactions within a disordered local moment (DLM) description of the paramagnetic state [3,4] and also, following Liechtenstein et al. [5], in terms of infinitesimal rotations on the basis of the magnetically ordered ground state.

## 2. Results and discussion

First, self-consistent calculations were carried out for each of the overlayer systems in terms of the scalar-relativistic spin-polarized screened Korringa–Kohn–Rostoker method [6]. No attempt was made to include lattice relaxations with respect to a perfect parent lattice of bulk copper. A detailed description of the magnetic moments as obtained from these calculations will be given elsewhere [7]. Hereby it is only worth to mention

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that in Co films the disordered local moments were, in general, 0.2–0.4$\mu_B$ smaller than those in the ferromagnetic state. In Ni films treated within the DLM picture, in many cases, layers with even zero magnetic moment were found. Although in the future it seems to be interesting to study the formation of such magnetically dead regions, what follows the DLM results on Ni films will be excluded.

For Co overlayers very similar exchange pair interactions from both types of calculations were obtained. Possibly due to an extra effective exchange field represented by the ordered spin-state, the NN interactions derived from the ferromagnetic state were, however, systematically larger in magnitude than calculated from the DLM state. In the monolayer case an opposite relation was found, which we attribute to the fact that the interfacial hybridization between Cu and Co states, decreasing the tendency to ferromagnetism of Co, is more pronounced in the ordered ferromagnetic state than in the magnetically disordered state.

Fig. 1 illustrates typical exchange pair interactions in the $Co_5$/Cu (0 0 1) and $Ni_5$/Cu (0 0 1) overlayers as sorted with respect to pairs of layers. Although in both overlayer systems the ferromagnetic (negative) NNIs dominate, especially for neighbor layers, one can notice also sizeable NNN interactions. Clearly, NNIs near the surface (5-5 and 4-5) are largest in magnitude, a fact which apparently correlates with the well-established trend to enhanced ferromagnetism at many metallic surfaces. At the interface of the Co film and Cu substrate a similar trend applies. The NNIs at the Ni–Cu interface (1-1 and 1-2) are, however, obviously smaller in magnitude than those even in the interior of the Ni film (3-3 and 3-4). This might be a consequence that the above mentioned interfacial hybridization is larger between Ni and Cu states than between Co and Cu states.

The Curie temperatures obtained within a mean-field approach are plotted in Fig. 2 together with experimental data. Since thermal fluctuations are expected to be increasingly important when the dimension of the system is

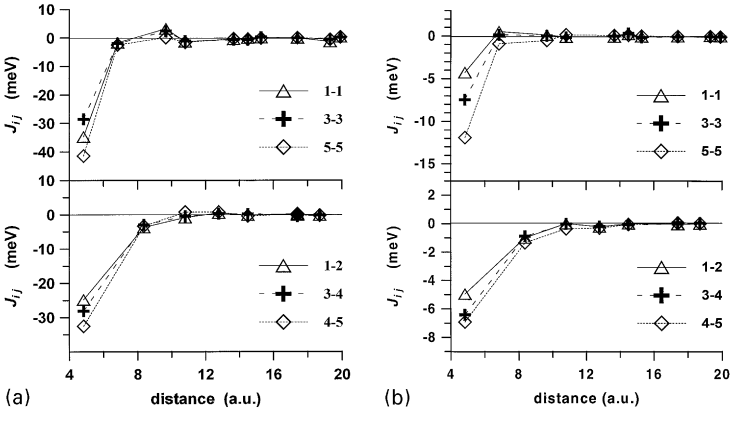


Fig. 1. Heisenberg parameters as calculated in terms of infinitesimal rotations for $Co_5$/Cu (0 0 1) (left panel) and $Ni_5$/Cu (0 0 1) (right panel) overlayers. In the legends the pair of numbers $p$–$q$ label the corresponding pair of layers. The labeling of the layers increases from the substrate toward the surface.

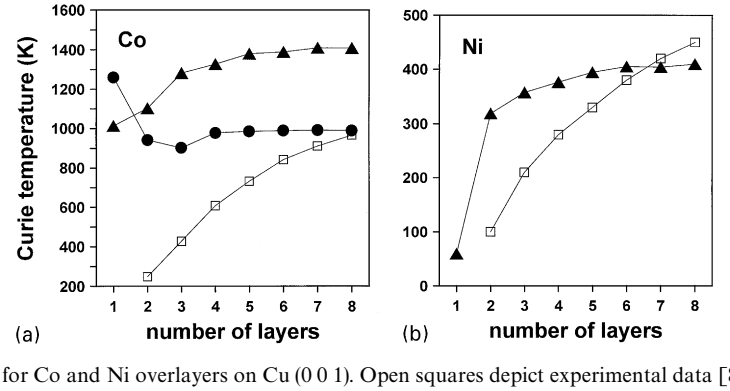


Fig. 2. Curie temperatures for Co and Ni overlayers on Cu (0 0 1). Open squares depict experimental data [8], while all other symbols display results of the mean-field approach by using Heisenberg parameters as calculated from the DLM state (filled circles) and from the ordered ground state (filled triangles). Solid lines serve as a guide for the eyes.

reduced, our results for $T_C$ should be regarded only as crude estimates. This is most pronounced for mono- and bilayers. Taking into account this general argument, the monotonous increase of $T_C$ with increasing film thickness is well reproduced. Since, as mentioned above, with exception of the monolayer case the exchange interactions derived from the ordered state are larger in magnitude than those calculated from the DLM state, for Co films a similar relation between the corresponding $T_C$'s can be seen.

In conclusion, we have shown that for thin Co films on Cu (0 0 1) the two methods provide a comparable description of the exchange pair interactions, while for Ni films only that in terms of infinitesimal rotations seems to be realistic.

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## References

[1] P.J. Jensen, H. Dreyssé, K.H. Bennemann, Europhys. Lett. 18 (1992) 463.
[2] K.J. Strandburg, D.W. Hall, C. Liu, S.D. Bader, Phys. Rev. B 46 (1992) 10818.
[3] A.J. Pindor, J. Staunton, G.M. Stocks, H. Winter, J. Phys. F 13 (1983) 979.
[4] B.L. Györffy, A.J. Pindor, J. Staunton, G.M. Stocks, H. Winter, J. Phys. F 15 (1985) 1337.
[5] A.I. Liechtenstein, M.I. Katsnelson, V.P. Antropov, V.A. Gubanov, J. Magn. Magn. Mater. 67 (1987) 65.
[6] L. Szunyogh, B. Újfalussy, P. Weinberger, J. Kollár, J. Phys. Rev. B 49 (1994) 2721.
[7] L. Udvardi, L. Szunyogh, submitted for publication.
[8] S.Z. Wu, F.O. Schumann, G.J. Mankey, R.F. Willis, J. Vac. Sci. Technol. B 14 (1996) 3189.