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# Hyperfine fields in Fe–Cr thin films

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**Abstract**

We have calculated the electronic structure of the 2Cr/3Fe/2Cr slab in bcc(1 1 0) geometry using FLAPW method in the local spin density approximation (LDA). The main aim of this work was to compare the calculated values of the hyperfine fields ($H_f$) with these obtained in the experiment carried out by Żukrowski et al. (J. Magn. Magn. Mater, 1995, 145, 97).

Our calculation shows the influence of the ordering on the Fe hyperfine fields and for the measured Cr/3.3Fe/Cr film we suggest the existence of two different $H_f$ values in each Fe plane, differing by 0.4–0.8 T. The magnetic moments of chromium are near 0.7 $\mu_B$ on the surface and oppositely oriented in the plane, while subsurface moments are small and anti-parallel to iron spins. The moments of iron atoms on the interface are slightly reduced. 

## 1. Introduction

The Fe/Cr system attracts great interest because of its interesting properties: the giant magnetostriction [2], the exchange coupling [3–7] and the oscillatory exchange coupling [8] to name but a few (for reviews see [9]).

The $^{57}$Fe-conversion electron Mössbauer spectroscopy (CEMS) [10, 11] is an excellent technique, allowing especially for the investigation of the local magnetic structure. Our work was stimulated by the experiment carried out by Żukrowski et al. [1] on the bcc (1 1 0) Cr/Fe/Cr sandwiches (see also [12]). In order to explain their experimental results, we have performed the electronic structure calculation on bcc (1 1 0) 2Cr/3Fe/2Cr system using an all-electron FLAPW method for thin films [13]. Our calculation shows that iron atoms should have two distinct values of the hyperfine fields in each layer. The anti-ferromagnetic chromium, even as a second neighbor, influences the fields on Fe atoms. The difference between the fields in one layer, although small (0.38, 0.78 T) seems to be significant (see discussion below). The obtained values for $H_f$ are smaller than the experimental ones, but it is probably due to the size effect (thin covering – only two layers of chromium – in our modeling calculation).

## 2. Details of calculations

We have performed the self-consistent electronic structure calculation using the FLAPW method. The real system is modeled by the 7-layer film (2Cr/3Fe/2Cr) of bcc (1 1 0) geometry. The lattice constant is taken as that of the pure iron ($a_0 = 5.417$ a.u.), as in our previous calculations [13]. This is a plausible assumption due to the very small mismatch between iron and chromium lattice constants (0.7%).

For the exchange-correlation potential we have used the parameterization scheme of Perdew–Zunger [14]. The wave functions in muffin-tin spheres were obtained in the scalar-relativistic approximation [13]. The Brillouin zone integration was performed using 16–36 magical $k_\parallel$ points. The hyperfine fields was obtained using a non-relativistic formula, to allow for comparison with our older results [15]. The convergence was assumed when the differences in hyperfine fields were smaller than 0.01 T.

We have not performed the energy minimization, thus fixing the geometry as described above, according to the experimental situation [1].

Our calculation was started with the superposed density of free atoms. The Cr atom was allowed to have initial antiferromagnetic configuration in both layers. The calculation was repeated , first starting from $d^5$ Cr

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configuration with total spin $S = 2$, then with $S = \frac{1}{2}$. The two calculations converged to the same final density. We think, that by allowing for system to stay in some metastable state with small antiferromagnetic admixture, we better simulated the real experimental samples, where the Cr covering was thick.

## 3. Discussion

The results of the calculation are summarized in Tables 1 and 2. From Table 1 one sees that in the surface layer of chromium the moments ($\sim 0.7$–$0.8\ \mu_B$, only small enhancement in comparison to bulk ) are aligned anti-parallel to each other, whereas in the interface they are small, parallel to each other but anti-parallel to the iron moments in agreement with the conclusion of Xu and Freeman [16, 17]. The iron moments are only affected at the interface. It is worthwhile to notice, that there is practically no charge transfer between atoms in the same layer.

Table 2 summarizes our results for the hyperfine field (only Fermi contact term included). Due to anti-parallel alignment of the chromium moments there are small but detectable differences in the fields on iron the atoms in the same layer. This is due to the delicate balance in the magnetic interactions of the constituent atoms (Fe–Fe, Fe–Cr, Cr–Cr) as discussed in [16]. The central layer $H_f$ is smaller than the bulk one in contrast to other investigated systems [15].

We compared our calculation with the CEMS measurements carried out by Żukrowski et al. [1]. Among the measured sandwiches, Cr/3.3Fe/Cr system – consisting of 3.3 monolayers of iron sandwiched between chromium – seems to be most suited. The experimentally obtained fields (25.8 and 34.8 T) are in quite a good qualitative agreement with ours (see Table 2). However, our calculation suggests that it should be *two* different fields in each iron layer for this system. The differences are $\sim 0.38$ T at the interface and $\sim 0.76$ T in the central layer. Theoretically, such differences could be resolved by the Mössbauer experiment, as the spectral resolution is about 0.3 T. The new analysis of the experiment [18] on the above mentioned system has shown only, that on the basis of the statistical analysis our model cannot be rejected. The poor resolution is probably due to imperfections, which are present at the iron-chromium interface in the real probe.

In conclusion, we calculated hyperfine fields for 2Cr/3Fe/2Cr slab, predicting two different fields in each iron layer. The present experiment does not allow to verify unambiguously our results.

Table 1
Charges and moments ($\mu_B$) in layers for 2Cr/3Fe/2Cr film: S – surface layer, C – central layer; ○ – Cr, ● – Fe denote positions of the given element in the 2-D elementary cell

| Layer | Atom | Spin ↑ | Spin ↓ | Moment | Total charge |
|---|---|---|---|---|---|
| S | Cr | 2.822 | 1.955 | 0.867 | 4.777 |
| | Cr | 2.033 | 2.744 | -0.710 | 4.777 |
| S-1 | Cr | 2.335 | 2.566 | -0.231 | 4.900 |
| | Cr | 2.440 | 2.460 | -0.020 | 4.900 |
| S-2 | Fe | 4.604 | 2.467 | 2.136 | 7.071 |
| | Fe | 4.567 | 2.508 | 2.059 | 7.075 |
| C | Fe | 4.709 | 2.316 | 2.393 | 7.026 |
| | Fe | 4.695 | 2.331 | 2.364 | 7.027 |

Table 2
Fermi contact term (in T) for Fe atoms in different layers; ● denotes position of the iron atom in the 2-D elementary cell

| Layer | Atom | Core | Valence | Total |
|---|---|---|---|---|
| S-2 | Fe | -26.14 | 1.72 | -24.42 |
| | Fe | -25.24 | 0.44 | -24.80 |
| C | Fe | -29.52 | -1.54 | -31.06 |
| | Fe | -29.21 | -1.07 | -30.28 |

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## References

[1] Żukrowski J, Liu G, Fritzsche H, Gradmann U. J Magn Magn Mater 1995;145:57.
[2] Baibich MN, Broto JM, Fert A, Nguyen Van Dau F, Petroff F, Etienne P, Creuzet G, Friederich A, Chazelas J. Phys Rev Lett 1988;61:2472.
[3] Grüberg P, Schreiber R, Pang Y, Brodsky MB, Sowers H. Phys Rev Lett 1986;57:2442
[4] Saurenbach F, Walz U, Hinchey L, Grünberg, P, Zinn, W, J Appl Phys, 1988;63:3473.
[5] Binasch G, Grünberg P, Saurenbach F, Zinn, W, Phys Rev B 1989;39:4828.
[6] Tomaz MA, Antel WJ, O'Brien WL, Harp GR, Phys Rev B 1997;55:3716.
[7] Freyss M, Stoeffler D, Dreyssé H, Phys Rev B 1997;56:6047.
[8] Stiles MD, Phys Rev B 1996;54:14 679.

[9] Fert A, Grünberg P, Barthelemy A, Petroff F, Zinn W. J Magn Magn Mater 1995;140–144: 1; In Heinrich B, Bland JAC, editors. Ultrathin magnetic Structures II, Ch. 2. Berlin: Springer, 1994;45.
[10] Korecki J, Gradmann U. Phys Rev Lett 1985;55:2491.
[11] Przybylski M, Gradmann U, Korecki J, J Magn Magn Mater 1987;69:199.
[12] Landes J, Sauer C, Brand RA, Zinn W, Mantl S, Kajcsos ZS. J Magn Magn Mater 1990;86:71.
[13] Karaś W, Noffke J, Fritsche L. J Chim Phys 1989;86:861.
[14] Perdew JP, Zunger A. Phys Rev B 1980;23:5048.
[15] Karaś W, Korecki J, Przybylski M, J Magn Magn Mater 1995;140–144:665.
[16] Xu J-H, Freeman AJ, J Magn Magn Mater 1990;86: 26.
[17] Xu J-H, Freeman AJ. Phys Rev B 1993;47:165.
[18] Żukrowski J. Private communication.