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Oscillatory interlayer magnetic coupling and induced magnetism in Fe/Nb multilayers

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Abstract. We present an *ab initio* calculation of interlayer magnetic coupling for Fe/Nb multilayers using the self-consistent full-potential linearized augmented-plane-wave (FLAPW) method. For this calculation, we have constructed supercells consisting of *bcc* Fe and Nb multilayers in Fe/Nb/Fe sandwich geometry stacked along (001) direction. In the supercells two Fe layers are separated by Nb layers ranging from 1 to 11 layers. We have calculated the total energy of the system as a function of Nb spacer layer thickness. For each spacer layer thickness, we have done three calculations corresponding to para, ferro and antiferromagnetic ordering of Fe atoms. The interlayer magnetic coupling is obtained from the energy difference of the systems in which Fe layers are antiferromagnetically and ferromagnetically ordered. We find that the interlayer magnetic coupling oscillates with increasing Nb spacer thickness in agreement with the experimental results. The induced magnetic moment is also found to be oscillating with increasing Nb spacer layer thickness.

Keywords. Interlayer magnetic coupling; GMR; DOS.

1. Introduction

During the last decade magnetic multilayers have received a lot of attention due to their interesting properties which are very different from the bulk properties. Magnetic multilayers show new phenomena like oscillating interlayer magnetic coupling (IMC) (Grunberg *et al* 1986; Parkin *et al* 1990; Unguris *et al* 1991) and giant magnetoresistance (GMR). Such oscillations in interlayer magnetic coupling and the saturation magnetoresistance were reported by Parkin *et al* (1990) with a period 15–20 Å in Fe/Cr, Co/Cr, Co/Ru multilayers. Purcell *et al* (1991) showed that the coupling oscillates with a smaller period of 3·0–4·0 Å in Fe/Cr/Fe sandwich structure. The first theoretical explanation was given by Bruno and Chappert (1991, 1992) within the Rudermann–Kittel–Kasuya–Yosida (RKKY) picture. They explained the interlayer coupling oscillation as a function of spacer layer thickness but in the limit of large spacer thickness. However, the coupling strength, J, in their work was described by an adjustable parameter. Thus to understand this phenomenon from the first principles an *ab initio* calculation is needed. The *ab initio* calculations of the exchange coupling, J, have been reported for various systems such as Fe/Cr, Fe/Cu, Fe/Mo, Co/Cu (Lang *et al* 1993; Mirbt *et al* 1995; Niklasson *et al* 1996). Recently combined theoretical–experimental work on Fe/Au superlattices (Yoshihara *et al* 2001) showed that IMC strength, J, exhibits oscillatory behaviour but the IMC was found to be ferromagnetic for all layers.

The experimental results for Fe/Nb multilayers (Mattson *et al* 1992) show oscillatory interlayer magnetic coupling as a function of Nb layer thickness with a period of 9·0 Å. Sticht *et al* (1991) showed the oscillating exchange coupling in Fe/Nb multilayers as a function of Nb spacer layer thickness using the augmented spherical wave (ASW) method (Williams *et al* 1979). However, the calculated period of oscillation was found to be half the experimental value. Probably this disagreement can be attributed to the ASA approximation. To ascertain this we have done a self-consistent full-potential linearized augmented-plane-wave (FLAPW) method (Blaha *et al* 1999) which treats crystal potential very accurately and makes no approximations like ASA. Our results show a period of 6·0 Å which is a substantial improvement over the ASW work (Williams *et al* 1979).

2. Computational details

All calculations reported in this paper are carried out using the self-consistent full-potential linearized augmented-plane-wave (FLAPW) method (Blaha *et al* 1999), within local spin density approximation (LSDA) in a scaler relativistic version without spin–orbit coupling. To perform this calculation we constructed tetragonal supercells consisting of *bcc* Fe and Nb multilayers in Fe/Nb/Fe sandwich structure along (001) direction. We have taken one Fe monolayer (ML) and the number of Nb monolayers are ranging from 1 ML to 11 ML in supercells. There is 13% lattice mismatch in pure Fe and Nb *bcc* structures. To reduce the lattice mismatch we have taken lattice constant equal to 3·12 Å, which is an average of pure Fe and Nb *bcc* lattice constants. The lattice

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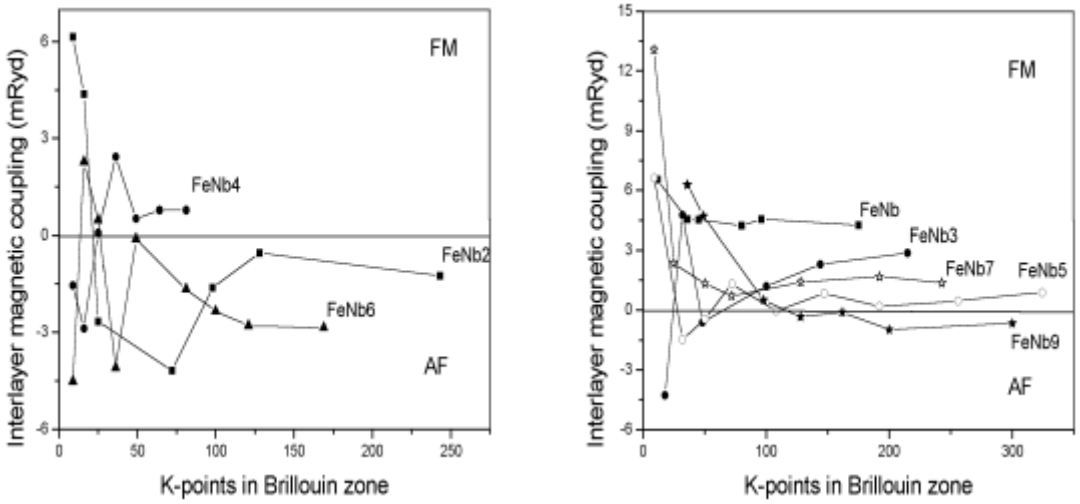

Figure 1. Exchange coupling, J (mRyd) for Fe/Nb multilayers as a function of k-points in Brillouin zone. The dots show the calculated results.

parameter along (001) direction changes from 3·12 Å to 18·72 Å in supercells. The muffin tin radii of Nb and Fe atoms are taken equal to 1·33 Å. For the calculation of the interlayer magnetic coupling, we calculated the total energy for ferro and antiferromagnetic ordering of Fe atoms for each Nb spacer layer thickness self-consistently. The interlayer magnetic coupling has a cosine dependence on the angle between adjacent Fe layers magnetization directions. To obtain the higher order coupling terms one has to consider noncollinear magnetic configurations. The total energy difference of ferro and antiferromagnetic configurations is proportional to the interlayer magnetic coupling. Thus the interlayer magnetic coupling, J, is defined as

$$J(d) = E_{\text{tot}}^{\uparrow\downarrow}(d) - E_{\text{tot}}^{\uparrow\uparrow}(d),$$

where d is the thickness of the spacer layer and $E_{\text{tot}}^{\uparrow\downarrow}$ and $E_{\text{tot}}^{\uparrow\uparrow}$ are the total energies of the multilayer in antiferromagnetic and ferromagnetic arrangements.

3. Results and discussion

We have calculated the total energy of multilayer for para, ferro and antiferromagnetic ordering of Fe atoms for each Nb spacer layer thickness. We find that the total energy for paramagnetic multilayer is always higher than the energy of the other two magnetic configurations. For the calculation of the total energy and magnetic coupling a sufficiently large number of k-points is needed as shown in figure 1. We see that convergence is reached if we use about 200 k-points. We find that the interlayer magnetic coupling converges faster than the total energy.

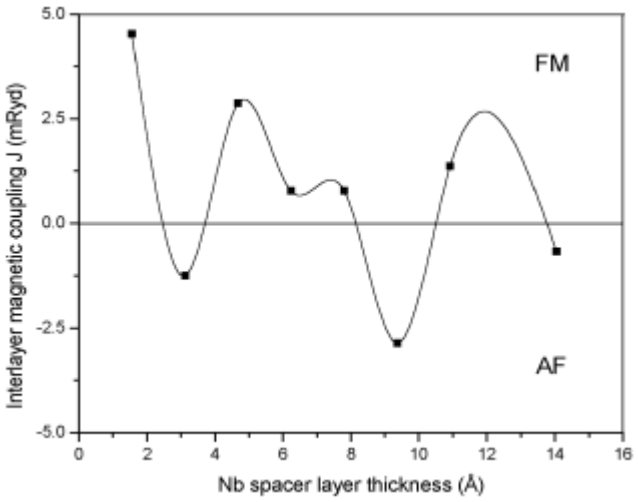

Figure 2. Exchange coupling, J (mRyd) for Fe/Nb multilayers as a function of Nb spacer layer thickness. The dots show the calculated results and the curve is a spline fit.

The interlayer magnetic coupling of Fe/Nb multilayer when varying the Nb space layer thickness is shown in figure 2, as a function of Nb spacer layer thickness. The interlayer magnetic coupling flips from ferromagnetic to antiferromagnetic at around 2·5 Å and 8·0 Å and then to ferromagnetic coupling at around 4·0 Å and 10·5 Å of Nb spacer. The period of oscillation is found to be ~6·0 Å which is close to the experimental result of 9·0 Å (Mattson *et al* 1992). This is a substantial improvement over the ASW work (Sticht *et al* 1991). The FLAPW method treats the potential much more accurately than the ASA (Williams *et al* 1979) and this may be the reason for getting an improved period of oscillation. This period may further improve if a better exchange correlation potential is used. Note that in our calculations we are

considering smooth interfaces but real systems are characterized by roughness. The period may further increase if we take care of the roughness (Bruno and Chappert 1991).

In table 1, we give DOS at Fermi level, total energy for several Fe/Nb multilayers in ferro and antiferromagnetic configurations. From this table we note an interesting correlation between oscillatory behaviour of the interlayer magnetic coupling and the DOS at the Fermi level. Table 1 shows that for a given Fe/Nb multilayer, the favourable magnetic configuration has smaller DOS at the Fermi level.

We find that Fe layers induce magnetic moments on Nb atoms. In figure 3, we show the induced magnetic moment per atom on Nb in spacer layers when Fe atoms are ferromagnetically ordered in 3Fe/9Nb multilayers system. It is interesting to see that the induced magnetic moments show oscillations although the amplitude of the oscillations away from the interface is quite small.

Table 1. DOS at the Fermi level, total energy for Fe/Nb multilayer in both magnetic configurations for 1–4 Nb spacer layers and interlayer magnetic coupling.

	Total DOS(e_f) states (eV)	Total energy (Ryd)	Interlayer magnetic coupling
FeNb (F)	4·19042	−20348·07652	F
FeNb (AF)	5·29611	−20348·07227	
FeNb2 (F)	6·49429	−35613·83541	AF
FeNb2 (AF)	5·46562	−35613·83594	
FeNb3 (F)	5·24787	−50879·61729	F
FeNb3 (AF)	6·63792	−50879·61442	
FeNb4 (F)	7·17330	−66145·36706	F
FeNb4 (AF)	7·93536	−66145·36624	
FeNb5 (F)	8·92182	−81411·11539	F
FeNb5 (AF)	9·11519	−81411·11462	
FeNb6 (F)	12·19656	−96676·86574	AF
FeNb6 (AF)	11·23548	−96676·86857	
FeNb7 (F)	14·30400	−111942·61322	F
FeNb7 (AF)	14·41399	−111942·61153	
FeNb9 (F)	19·72510	−142474·10721	AF
FeNb9 (AF)	18·83929	−142474·10755	

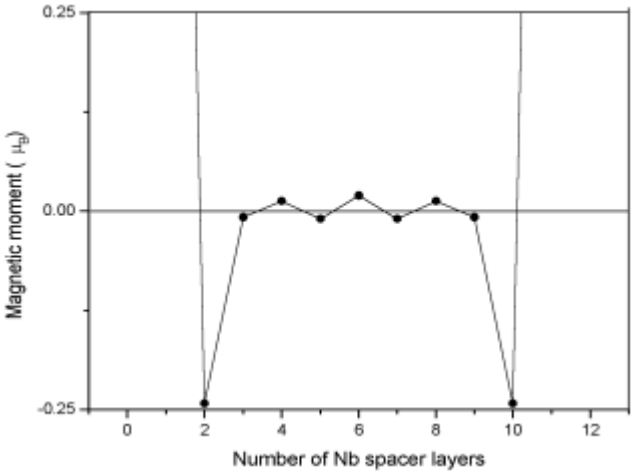

Figure 3. The induced magnetic moment on Nb spacer layers in 3Fe/9Nb multilayer. The dots show the calculated results. The Fe atoms are placed at positions 0, 1 and 11.

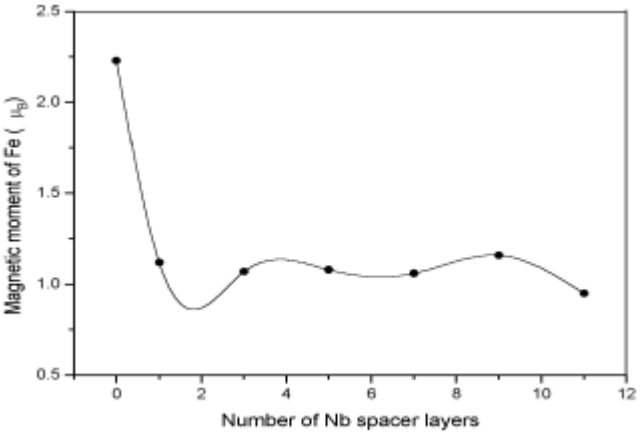

Figure 4. The magnetic moments on Fe atoms in Fe/Nb multilayers as a function of Nb spacer layers. The dots show the calculated results and the curve is a spline fit.

In figure 4, we show the change in the magnetic moment per atom in Fe layers as a function of Nb spacer layers and find that it also shows oscillations. The magnetic moment of Fe is reduced at the interface as compared to the bulk value. The magnetic moment of Fe changes between 1·30 to 1·00 μ_B which is smaller than the magnetic moment in bulk Fe(2·24 μ_B). If we consider the reduction in the magnetic moment of Fe due to the decrease in number of Fe neighbours from 8 to 4, a slightly larger value of magnetic moment is obtained. The reduction in magnetic moment of Fe atoms at interface depends on Nb spacer thickness and magnetic moment of Nb spacer layers also depends on Fe layer thickness. This is a consequence of the change in hybridization between the Fe–Fe *d* bands and Fe–Nb *d* bands (Stoeffler *et al* 1994).

4. Conclusions

We have calculated the exchange coupling between Fe layers when separated by Nb spacer layers using the self-

consistent FLAPW method. We observe an oscillating exchange coupling as a function of Nb spacer layer thickness with a period of 6·0 Å. We find that the induced magnetic moments on Nb atoms and Fe atoms oscillate as a function of Nb spacer layer thickness. We also find an interesting correlation between the interlayer magnetic coupling and the density of states at the Fermi level.

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