Bull. Mater. Sci., Vol. 22, No. 4, June 1999, pp. 761–763. © Indian Academy of Sciences.

GMR in Ni/Cu multilayers: an electronic structure study

S K GHOSH, H G SALUNKE†, G P DAS†*, A K GROVER and M K TOTLANI
Materials Processing Division, †Technical Physics and Prototype Engineering Division,
Bhabha Atomic Research Centre, Mumbai 400 085, India

MS received 6 January 1999

Abstract. ***Ab initio*** **self-consistent semi-relativistic spin-polarized TB-LMTO energy band calculations have been carried out on Ni/Cu(100) multilayers, to study the in-plane as well as perpendicular to plane giant magnetoresistance (GMR) effects. The magnetic interaction energies, evaluated as a function of layer thickness, indicate that the antiferromagnetic ordering is a possible ground state for manifestation of GMR. Using the density of states at Fermi level and the Fermi velocity, GMR has been estimated as a function of the Cu spacer thickness.**

Keywords. **Multilayers; electronic structure; giant magnetoresistance.**

1. Introduction

Occurrence of giant magnetoresistance (GMR) in magnetically coupled multilayers has been a topic of intense activity in recent times (Levy 1994). Since the discovery of GMR in Fe/Cr system (Baibich *et al* 1988), several experimental and theoretical studies have been reported to elucidate its microscopic origin. It is now understood that if an otherwise ferromagnetic (FM) material can be coupled antiferromagnetically (AFM) by some mechanism, then such multilayers show large drop in magnetoresistance on application of relatively small magnetic field. However, these antiferromagnetic coupling can be brought about by different microscopic processes. For instance, the origin of GMR in Fe/Cr multilayers is due to proximity effect of Cr on ferromagnetic Fe (Parkin *et al* 1990), while in multilayers such as Ni/Cu, Co/Cu etc it is the RKKY superexchange which cause a weak antiferromagnetic alignment in Ni and Co layers respectively (Bruno 1995). Bird and Schlesinger (1995) first convincingly demonstrated that if the thickness of Cu layer is suitably adjusted in electrodeposited Ni–Cu multilayers, then the ground state is AFM instead of being FM. The RKKY type GMR oscillations in Ni/Cu multilayers have been experimentally measured by several workers (Schwarzacher and Lashmore 1996). There was a controversy about the existence of magnetically dead Ni layers at the interface, which was first resolved by Jarlborg and Freeman (1980). However, to date there has been no systematic attempt to understand from first principles the exact nature of the interlayer magnetic coupling and GMR in Ni/Cu(100) system. This is precisely the aim of the present work.

2. Method of calculation

We have carried out self-consistent supercell energy band calculations using tight-binding linear muffin tin orbital (TB-LMTO) method within the atomic sphere approximation (ASA) (Andersen and Jepsen 1984). Spin-averaged as well as spin-polarized (FM and AFM)** calculations were performed using local density (LDA) and local spin density (LSDA) exchange-correlation potentials respectively. The actual multilayer system has been modelled by a $(m + n)$ supercell with m layers of Ni and n layers of Cu periodically repeated along the (100) direction (call it z-direction). Starting with the smallest (3 + 3) supercell calculation, we have gone to (5 + 7) and (7 + 5) supercells by increasing the number of Ni and Cu layers progressively, in order to monitor the various electronic and magnetic properties as a function of the layer thickness or cell size. Both Ni and Cu being fcc, the supercells have tetragonal structure. Although Ni and Cu have a lattice mismatch of ~ 2·5%, we have chosen the nearest neighbour Ni–Ni, Cu–Cu and Ni–Cu distances to be the same (viz. 2·49 Å) in the supercells considered. No structural relaxation has been taken into account. All our calculations are semi-relativistic, and with frozen-core approximation. We have used s, p and d partial waves on all the spheres and included the combined correction term. Since the supercells here are all closely packed, the atomic sphere overlaps (≤ 15%) are well within the permissible limit of ASA. The supercell calculations are done using 15 k-points each along x and y-direction (basal plane) and 2 k-points along

*Author for correspondence
**For AFM case the unit cell is doubled and the spin directions in consecutive cells are reversed; for the sake of uniformity in k-mesh etc. we have performed the corresponding FM calculation also in the same cell.

the z-direction (114 k-points in the irreducible Brillouin zone).

3. Results and discussion

The site as well as spin-projected partial densities of states (DOS) for the (3 + 3), (5 + 7) and (7 + 5) Ni/Cu(100) supercells reveal many detailed features of the electronic structure of this system. The central Cu and Ni atoms show bulk-like behaviour with three separate bonding, non-bonding and anti-bonding peaks in DOS. The interface atoms show a more broadened DOS with less structure, mainly because of the hybridization, although the distinguishability between Cu-like and Ni-like features are still retained. Also the interfacial DOS's are shifted towards the supercell Fermi level because of the interface-induced dipole caused by the charge transfer between Cu and Ni atoms. For each panel in the FM and AFM partial DOS's one finds a relative shift between the majority (up) and the minority (down) spin, which leads to the manifestation of magnetic moment in that atomic layer. Of particular interest here are the results for the AFM state. Figures 1 and 2 respectively show the variations of the charge transfer and the magnetic moment across the multilayer thickness. As expected, the central layers of Ni and Cu in (7 + 5) and (5 + 7) supercells respectively tend to achieve the bulk values of charge transfer and magnetic moment, in contrast to the (3 + 3) case. The Ni layer right at the interface gains a significant amount of charge at the cost of its neighbouring Cu as well as Ni layer (see figure 1).

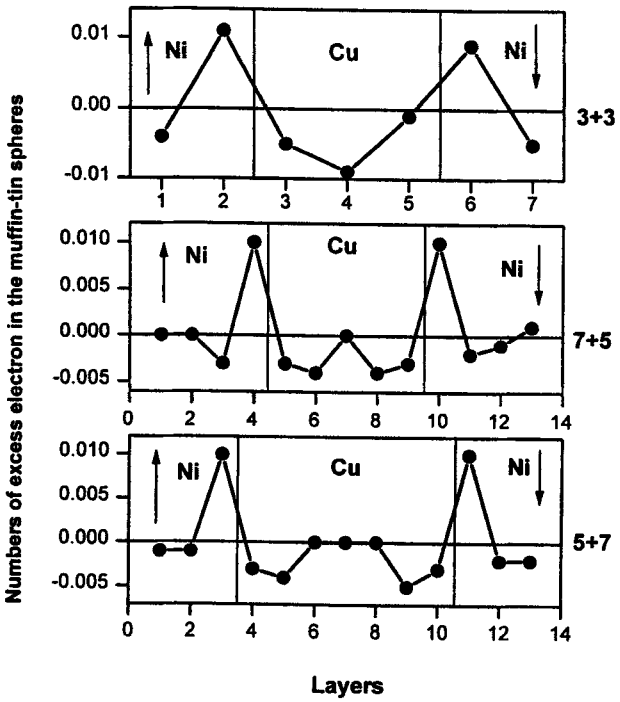

Figure 1. Charge transfer across the antiferromagnetically coupled Ni/Cu(100) multilayer.

As one goes deeper into the Ni layers, the excess charge tends to show Friedel oscillations (figure 1), while the magnetic moment does not (figure 2). As required for a RKKY superexchange the Cu layers do show a slight charge polarization for the eventual AFM ordering between the Ni layers. Also the interface Ni layers have a lower magnetic moment than the bulk value, in confirmation with expected norm (Jarlborg and Freeman 1980). Our results on the energetics, charge transfer and magnetic moment are in good agreement with earlier studies, giving us confidence for further predictions on the GMR of these materials.

Table 1 gives the magnetic interaction energy E_{mag} (MeV/atom) which has been defined for a $(m + n)$ multilayer as

$$E_{Mag} = \frac{E_{Tot}^{spin-av} - E_{Tot}^{spin-pol}}{m+n}. \quad (1)$$

We find that within the accuracy of our calculational method, the magnitudes of E_{mag} for FM and AFM state are comparable, although the later energy is always found to be lower. This confirms that the AFM ordering can indeed be a possible ground state for manifestation of GMR, as has been testified by experiments. Also our results show the magnetic interaction energy for the (7 + 5) supercell is the lowest, implying the highest relative stability.

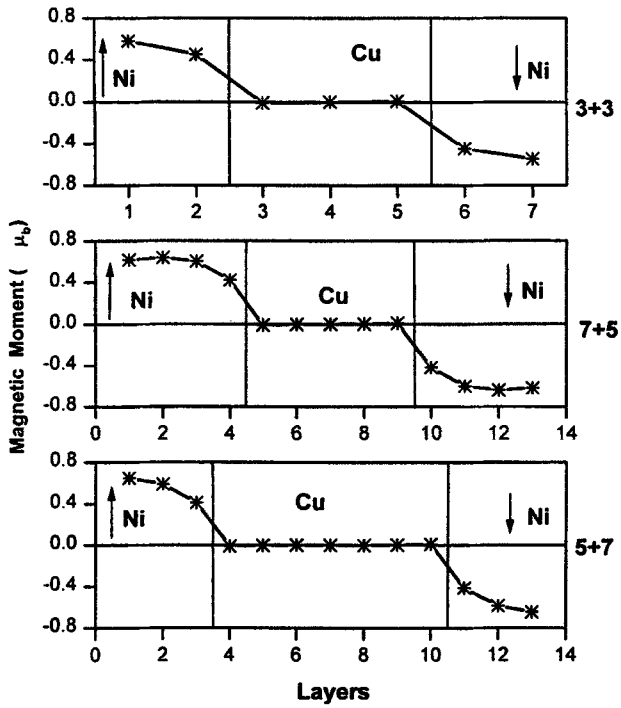

Figure 2. Variation of magnetic moment as a function of layer thickness in antiferromagnetically coupled Ni/Cu(100) multilayer.

Table 1. Magnetic interaction energy, E_{mag} (meV/atom) for the three structures studied.

Supercell	3 + 3	7 + 5	5 + 7
FM	− 13·0	− 28·2	− 24·4
AFM	− 14·0	− 28·3	− 25·3

Table 2. Comparison of calculated value of GMR with that measured from experiment.

% GMR	*i–p*	*p–p*	Expt
3 + 3	24·18	37·05	~ 2
7 + 5	41·21	69·11	7
5 + 7	29·90	58·76	~ 5

4. Giant magnetoresistance

The GMR in a magnetic multilayer is defined as:

$$\mathrm{GMR} = (\sigma^{\mathrm{P}} - \sigma^{\mathrm{AP}})/\sigma^{\mathrm{P}}, \tag{2}$$

where σ^{P} and σ^{AP} are the conductivity of the parallel and anti-parallel configurations respectively. We calculate conductivity using semiclassical Boltzmann transport equation under relaxation time approximation (Kai *et al* 1998). If the relaxation time in the Boltzmann transport equation is assumed to be independent of the wave vector $\bar{k}$, then the expression for conductivity is written as,

$$\sigma = e^2 D(\varepsilon_{\mathrm{F}}) v_{\mathrm{F}}^2 \tau, \tag{3}$$

where $D(\varepsilon_{\mathrm{F}})$ is the density of states at Fermi level (ε_{F}) and (v_{F}) is the Fermi velocity of the electrons. The Fermi velocity is defined as

$$v_{\mathrm{F}}^{\mathrm{AP(P)}} = \left(\frac{\sum_k v(\bar{k}) v(\bar{k}) \delta(\varepsilon_{\mathrm{AP(P)}}(k) - \varepsilon_{\mathrm{F}})}{\sum_k \delta(\varepsilon - \varepsilon_{\mathrm{F}})} \right)^{\frac{1}{2}} \tag{4}$$

The group velocity, $v(\bar{k})$, can be obtained from the energy gradient of the band as

$$v(\bar{k}) = \frac{1}{\hbar} \frac{\partial}{\partial k} \varepsilon(\bar{k}). \tag{5}$$

It is noted that since the electron mean free path for Cu (~ 93 Å) is greater than the spacer Cu width, the Ni/Cu multilayer is expected to show in-plane GMR due to interface scattering effects. In table 2 we present results for the in-plane (i–p) as well as perpendicular to the plane (p–p) GMR for the Ni/Cu multilayer. Our results show the same trend as that observed by others (Bird and Schlesinger 1995; Schwarzacher and Lashmore 1996). However, the calculated values overestimate the measured values, as confirmed by other theoretical calculations published. This is partly due to the inaccuracies in the method of calculation and partly due to the simplifications used in calculation of conductivity of the multilayer.

5. Conclusion

In conclusion, we find that the magnetic interaction energy of the antiferromagnetically coupled Ni/Cu(100) multilayer competes with the ferromagnetically ordered multilayer, suggesting that AFM is indeed the possible ground state of this interesting system. Our results on interface Ni magnetic moment conform with the published works and that charge transfer from Cu to Ni shows Friedel oscillations as expected. The GMR calculated within the relaxation time approximation, show RKKY behaviour with (7 + 5) multilayer showing the largest GMR. These results agree qualitatively with the measurements on electrodeposited Ni/Cu multilayers.

Acknowledgement

We thank Drs A K Suri, S Banerjee and V C Sahni for encouragement and support of this work.

References

Andersen O K and Jepsen O 1984 *Phys. Rev. Lett.* **53** 2571

Baibich M N, Broto J M, Fert A, Nguyen V D, Petroff P, Etienne P, Creuzet G, Friederich A and Chazelas J 1988 *Phys. Rev. Lett.* **61** 2472

Bird K D and Schlesinger M 1995 *J. Electrochem. Soc.* **142** L65

Bruno P 1995 *Phys. Rev.* **B52** 411

Jarlborg T and Freeman A J 1980 *Phys. Rev. Lett.* **45** 653

Kai T, Ohashi Y and Shiiki K 1998 *J. Mag. Mag. Mater.* **183** 292

Levy P M 1994 in *Solid state physics* (eds) H Ehrenreich and D Turnbull Vol. 47, p. 367

Parkin S S P, More N and Roche K P 1990 *Phys. Rev. Lett.* **64** 2304

Schwarzacher W and Lashmore D S 1996 *IEEE Trans. Magn.* **32** 3133