

Piece-wise Potential Approach to Electronic Transport in Metallic Superlattice

J. I. Uba^{1,*}, A. J. Ekpunobi² and P. I. Ekwo²

¹*Nwafor Orizu College of Education, Onitsha, Anambra, Nigeria*

²*Nnamdi Azikiwe University, Awka, Anambra, Nigeria*

Metallic super-lattice is described in terms of piece-wise potential. With this scheme, a Drude-like resistivity model is developed, which applies to current-in-plane and current-perpendicular to plane transport. It shows that magnetic field perturbs the trajectory of itinerant electrons and the total structure potential, leading to helical Fermi surface in metallic superlattices. The model gives antiparallel state resistivity of $54.2 \mu\Omega\text{cm}$ in comparison to $54 \mu\Omega\text{cm}$ for $\text{Fe}_{30}\text{\AA}/\text{Cr}_{90}\text{\AA}_{40}$ reported by Baibich et al. (1988) and $19.7 \mu\Omega\text{cm}$ against $20.3 \mu\Omega\text{cm}$ at 2 GPa for $\text{Co}_{10}\text{\AA}/\text{Cu}_{10}\text{\AA}_{15}$ by Oomi et al. (1997). Results of the implementation on Co/Cu(Cr) structures show Co/Cr to be a better magneto-resistive structure.

1. Introduction

Electronic transport in metallic superlattices (MSLs) has been modelled in classical and quantum formalisms. Both address parallel and perpendicular transports to explain the current-in-plane (CIP) and current-perpendicular-to plane (CPP) giant magnetoresistance (GMR). The classical formalism rests upon the Boltzmann transport scheme and has yielded several resistivity formulae for CIP [1-4] and CPP [5] GMR. The Kubo and the Landauer-Buttiker formalisms form the main bases of quantum methods [6-9]. Despite variance in resistivity formulae, classical and quantum methods adopt series resistor model in the homogeneous limit $l_{j,\alpha} \gg a_j$ for CIP and CPP GMR [7], where $l_{j,\alpha}$ is mean free path in the j^{th} layer of electron of spin α and a_j is thickness of layer. As a result, CIP and CPP formulae rest on Ohm's law to which they all reduce to. For instance, the Boltzmann approach to CIP by Hood and Falicov [2] and CPP by Valet and Fert [5] and the Kubo formalism method of Camblong [6, 7].

In the established literature, there are myriads of different parameters that characterize CIP and CPP transport. These arise as a consequence of methods of development and in turn obscure validity of Drude formalism for electric conductivity in metals to which Ohm's law is associated. In some cases, the Drude formalism comes out as limiting law at large number of layers [9]. In light of this, and the fact that in homogeneous limit, the mean free path averages all sorts of scattering [7], it is reasonable to suggest

that a Drude-like description of spin-dependent transport would reduce the necessary parameters to mean free paths and relaxation times. The magnitude of both parameters would of course differ in the CIP and CPP since the effective electric field is not the same in both geometries.

It will be noted that transport in metallic superlattices is about an electron experiencing different scattering rates in different regions as it propagates through the entire structure [7]. This allows modelling of the metallic environment as a piece-wise constant potential (PCP). This paper aims at developing, in the frame of PCP, a Drude-like resistivity model that applies to both CIP and CPP geometries.

2. Method

2.1. Hamiltonian of the system

To proceed, the following assumptions are necessary.

- i. The main scattering mechanism is spin-dependent potential in bulk of metal [4].
- ii. Each metal layer presents a different spin-dependent crystal potential, so electrons are in the metallic environment with varying potentials. Therefore, a superlattice is assumed to be a single metal with piece-wise constant potentials, where interfaces are points of discontinuity.
- iii. No preference is made to either current-in-plane or current-perpendicular-to-plane geometry since the same parameters (but with different magnitude) would determine resistivity in either of the geometries.

*ikemuba@gmail.com

Consider a N-layered structure of thickness L, consisting of ferromagnetic and normal metals (Fig. 1), where $j=1, 2, 3, \dots, N$ is the layer index.

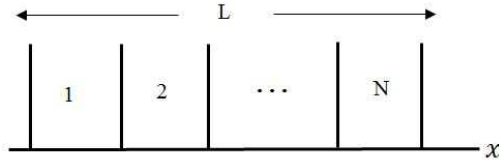


Fig.1: Schematic of superlattice. $J = 1, 2, 3, N$ denotes layers of ferromagnetic and normal metals in alternation. x is direction of layering.

In any of these layers, an electron of spin α ($\alpha = \uparrow$ or $\downarrow$), experiences a spin-dependent bulk potential $u_{j\alpha}$. So a layer is modelled after a potential well. If interfaces are neglected, the Hamiltonian of an electron of mass M_α traversing the super-lattice in the direction of layering

$$H_{0\alpha} = \frac{-\hbar^2}{2M_\alpha} \frac{d^2}{dx^2} + \sum_{j=1, \alpha}^N u_{j\alpha} \quad (1)$$

With the second assumption it is easy to account for interface by considering potential steps and s-d scattering potentials at points of discontinuity. The latter may be necessary because of inter diffusion during fabrication. So the system's Hamiltonian

$$H_\alpha = H_{0\alpha} + v_\alpha \quad (2)$$

Where, v_α is sum of potential steps a_α and s-d scattering potentials γ_α . Both are defined at i^{th} interface as

$$a_\alpha = u_{j,\alpha} - u_{j+1,\alpha} \quad (3)$$

and

$$\gamma_\alpha = \gamma_{\alpha i} \quad (4)$$

So for R number of interfaces

$$a_\alpha = \sum_{\alpha, i=1}^R (u_{j,\alpha} - u_{j+1,\alpha})_i \quad (5)$$

$$\gamma_\alpha = \sum_{\alpha, i=1}^R \gamma_{\alpha i} \quad (6)$$

The s-d potential may be chosen arbitrarily as long as it is small compared to potential steps. From the last two equations,

$$v_\alpha = \sum_{\alpha, i=1}^R (a_\alpha + \gamma_\alpha)_i \quad (7)$$

Hence Eqn. (2) becomes

$$H_\alpha = \frac{-\hbar^2}{2M} \frac{d^2}{dx^2} + \Lambda_\alpha \quad (8)$$

Where, $\Lambda_\alpha = u_\alpha + v_\alpha$ is the effective bulk potential seen by the electron. As the electrons are confined within the superlattice of total thickness L, the potential

$$\chi_\alpha = \begin{cases} \infty, & 0 < 0 \\ \Lambda_\alpha, & 0 \leq x \leq L, \\ \infty, & 0 > L \end{cases} \quad (9)$$

Eqns. (8) and (9) give a wave function similar to that of particle in a box. That is,

$$\Psi_\alpha = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad (10)$$

And, the kinetic energy

$$\begin{aligned} \epsilon_\alpha &= E - \Lambda_\alpha \\ &= \frac{n^2 \pi^2 \hbar^2}{2M_\alpha L} \end{aligned} \quad (11)$$

The quantum number is spin independent because of the energy degeneracy of the itinerant electron at Fermi level, $E_F = E$. However, their kinetic energies differ by the effective electron mass M_α due to spin dependent bulk potential.

2.2. Resistivity of the system

External electric field ϵ introduces additional energy to ϵ_α . So, at any instance, the electron's velocity is the sum of Fermi and drift velocities. The average value of which is given by the matrix element of the velocity operator, $\hat{V} \left(= \frac{-i\hbar}{M_\alpha} \frac{d}{dx} \right)$, will be zero since the electron might as well be moving in opposite directions. So, for the non-zero value, leads to drift velocity, it is reasonable to consider matrix element of square of the velocity operator. Thus,

$$\begin{aligned}
 \langle V_\alpha^2 \rangle &= \langle \Psi_\alpha | \hat{V}_\alpha^2 | \Psi_\alpha \rangle \\
 &= \frac{\hbar^2 k_\alpha^2}{M_\alpha^2} \\
 &= \frac{2\epsilon_\alpha}{M_\alpha^2} \quad (12)
 \end{aligned}$$

Here k_α is a wave vector different from Fermi vector. As $\langle V_\alpha^2 \rangle$ is tied to kinetic energy ϵ_α , Eqn. (12) gives the spin-dependent drift velocity

$$\begin{aligned}
 V_{d\alpha} &= \frac{\hbar k_\alpha}{M_\alpha} \\
 &= \frac{e\epsilon}{M_\alpha} \tau_\alpha \quad (13)
 \end{aligned}$$

Where, e is electronic charge and τ_α is the relaxation time, predominantly determined by Fermi velocity since $V_{d\alpha}$ is small in comparison.

On account of τ_α being determined by Fermi velocity, an electron incident on an interface may be described by Fig. 2 in which $V_{F\alpha}$ is Fermi velocity and $V_{Fy\alpha}$ and $V_{Fx\alpha}$ are the components, and β_α is the incidence angle.

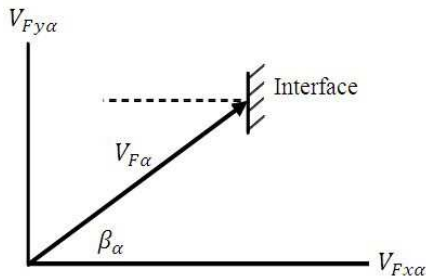


Fig.2: Trajectory of electron incident on an interface. $V_{Fy\alpha}$ and $V_{Fx\alpha}$ are components of Fermi velocity $V_{F\alpha}$. $V_{Fx\alpha}$ is in the direction of layering.

From Fig. 2 and using $V_F = \hbar k_F / M$,

$$V_{Fx\alpha} = V_{F\alpha} \cos \beta_\alpha \quad (14)$$

$$k_{Fx\alpha} = k_{F\alpha} \cos \beta_\alpha \quad (15)$$

Where, $k_{F\alpha}$ is the effective Fermi vector on the super-lattice and $k_{Fx\alpha}$ the component in direction of layering. Along the x-axis, the mean free path $l_{x\alpha} = V_{Fx\alpha} \tau_\alpha$. Thus

$$V_{d\alpha} = \frac{e\epsilon}{M_\alpha} \frac{l_{x\alpha}}{V_{Fx\alpha}} \quad (16)$$

If n_α is density of electrons of spin α assumed isotropic, then the corresponding current density is

$$\frac{I_\alpha}{A} = J_\alpha = \frac{n_\alpha e^2 \epsilon l_{x\alpha}}{M_\alpha V_{Fx\alpha}} \quad (17)$$

Where, A is the planar area of the super-lattice. It follows that contribution of spin α to the global resistivity has a Drude-like form

$$\rho_\alpha = \frac{M_\alpha V_{Fx\alpha}}{n_\alpha e^2 l_{x\alpha}} \quad (18)$$

It can be shown (Appendix A) that $n_\alpha = k_{F\alpha}^3 / 6\pi^2$. Using this, Eqn. (14) and $V_F = \hbar k_F / M$, yield the alternative form

$$\rho_\alpha = \frac{3\pi\hbar \cos \beta_\alpha}{k_{F\alpha}^2 e^2 l_{x\alpha}} \quad (19)$$

This illustrates the angular dependence of resistivity. In the magnetic field, this angle must change if there would be change in resistivity and leads to changes in $l_{x\alpha}$ and τ_α . The equation takes on a more tractable form when the substitution $l_{x\alpha} = V_{F\alpha} \tau_\alpha \cos \beta_\alpha$ is made. That is,

$$\rho_\alpha = \frac{3\pi\hbar}{k_{F\alpha}^2 e^2 l_\alpha} \quad (20)$$

Where, $l_\alpha = V_{F\alpha} \tau_\alpha$ is mean free path in the structure. This form is similar to Bauer's model [9], which is based on Landauer-Buttiker formalism. The Bauer's model is also similar to the model of Zhang and Levy [8]. The factor of 2 in Bauer's model is absent in the present contribution due to the spin asymmetry of Fermi vector (Appendix A) implemented herein. Finally, the global resistivity is simply given by summation of contributions of the two spin channels

$$\rho = \sum_{\alpha=\uparrow,\downarrow} \rho_\alpha \quad (21)$$

Furthermore, when the number of electrons of spin α , $N_\alpha = n_\alpha L$ is used with the approximation $M = M^\uparrow = M^\downarrow$, it follows from Eqns. (18) and (20) that

$$GMR = 1 - \frac{\tau_{AP}}{\tau_P} \quad (22)$$

Where, τ_{AP} is relaxation time in absence (antiparallel state) of magnetic field and τ_P is

relaxation time in the presence (parallel state) of magnetic field. In experiments, the magnetic field with respect to current can be in-plane or perpendicular to plane but it is never perpendicular to Fermi velocity due to the incidence angle. So in analogy with the classical motion of charge in a magnetic field, the conduction electrons would move in helical path as they traverse the structure.

3. Applications and Discussion

The form of the model used is Eqn. (20), which is implemented in a Python program with reasonable choices of τ_{AP} and τ_P . The case of spin independent effective mass and relaxation times is considered in this paper. First, functionality of the model is checked by implementing it on $\text{Fe30}\text{\AA}/\text{Cr9}\text{\AA}|_{40}$ [10] and $\text{Co10}\text{\AA}/\text{Cu10}\text{\AA}|_{15}$ [11]. The zero field (antiparallel state) resistivities of these superlattices in CIP geometry are $54.0\mu\Omega\text{cm}$ and $20.3\mu\Omega\text{cm}$ (at 2GPa), respectively. To apply the model, it is necessary to deduce observed parallel state resistivities from reported GMRs and then make an appropriate choice of system parameters. Second, we consider arbitrary $\text{Co(t)}/\text{Cu}(\text{Cr})15\text{\AA}|_6$ structures.

$$\text{Fe30}\text{\AA}/\text{Cr9}\text{\AA}|_{40}$$

The following parameters are chosen for this system:

- Anti-parallel relaxation time: $\tau_{AP} = 2.4 \times 10^{-10}\text{s}$;
- Effective electron mass: $4 \times$ free electron mass;
- Potentials [2]: $U_{Cr}^{\uparrow,\downarrow} = -5.77\text{ eV}$, $U_{Fe}^{\uparrow} = -8.23\text{ eV}$, $U_{Fe}^{\downarrow} = -5.73\text{ eV}$;
- s-d scattering potential for: up spin = 0.1 eV , down spin = 0.5 eV .

Our choice of τ_{AP} gives $54.20\mu\Omega\text{cm}$ zero field resistivity. Table 1 lists the parallel state resistivities. Figs. 3-5 show the GMR, parallel state resistivity as a function of parallel state relaxation time and the parallel state resistivity as a function of magnetic field.

Table 1: Magnetoresistance and parallel state resistivity of $\text{Fe30}\text{\AA}/\text{Cr9}\text{\AA}|_{40}$.

H(T)	*GMR	Resistivity ($\times 10^{-7}\Omega\text{m}$)	
		**Expt.	Theory
4.00	0.94	0.324	0.324
7.00	0.87	0.702	0.756
10.00	0.82	0.972	0.972
14.00	0.69	1.67	1.72
17.00	0.60	2.16	2.21
20.00	0.54	2.48	2.59
24.00	0.54	2.48	2.59
30.00	0.54	2.48	2.59
34.00	0.54	2.48	2.59
40.00	0.54	2.48	2.59

*From the GMR curve in the relevant literature.
**Deduced from reported *GMR.

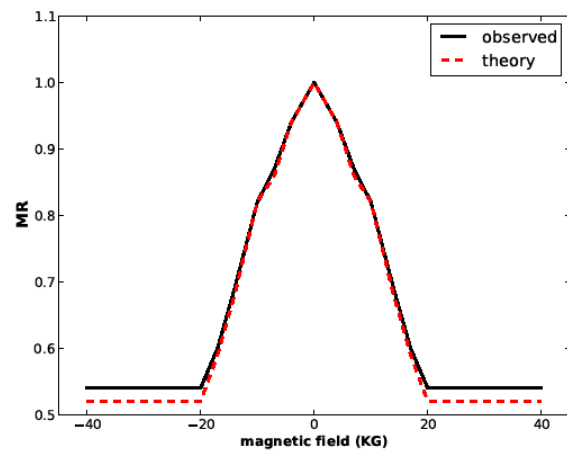


Fig.3: GMR of $\text{Fe30}\text{\AA}/\text{Cr9}\text{\AA}|_{40}$: Observed and calculated (observed values from [10]).

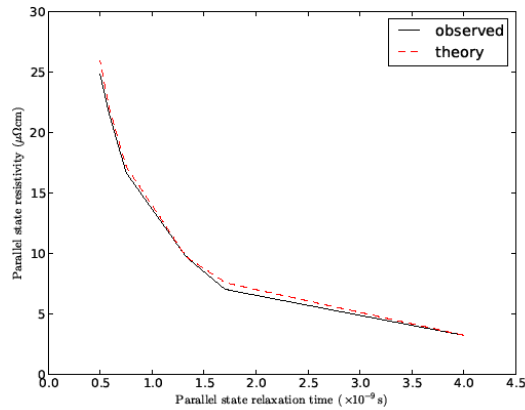


Fig.4: Experimental and theoretical parallel state resistivity of Fe30Å/Cr9Å₄₀ superlattice as function of parallel state relaxation time. (Experimental values deduced from [10]).

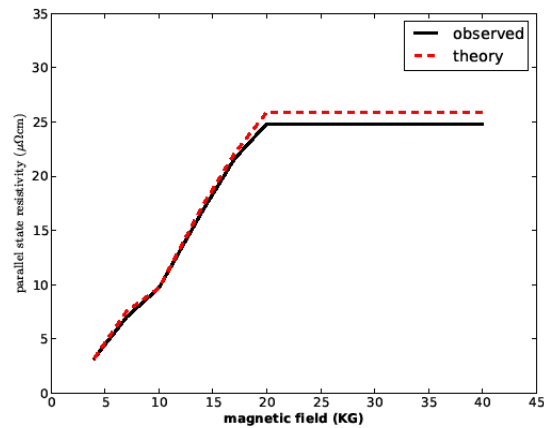


Fig.5: Experimental and theoretical parallel state resistivity of Fe30Å/Cr9Å₄₀ super-lattice as a function of magnetic field. (Experimental values after [10]).

It is observed from Fig. 3 that the model reproduced the GMR of the involved system. The discrepancies at higher $\mathbf{B}$ are primarily due to the choice of parallel state relaxation time τ_p . The increase in parallel state resistivity as depicted in Table 2 is a clear indication of the existence of additional potential due to $\mathbf{B}$ and perturbation of electron incident angle. The combined effect results to small τ_p for large resistivity (Fig. 4) at high magnetic field that attains constant value at saturation field as shown in Fig. 5. In comparison, τ_p at and beyond saturation field is about twice the antiparallel (zero field) relaxation time. This is expected since the Drude-like model is inversely

proportional to relaxation time and the parallel state resistivity at saturation field is nearly half the zero field resistivity as related by Baibich et al. [10] and observed in GMR experiments.

Electrical resistivity of a material is determined by the amount of scattering due to combined effect of crystal potentials, defects and interstitial atoms. Method of preparation and prevalent conditions determine crystal defects and interstitial atoms. So given a material fabricated via a certain technique, the electrical resistivity changes when the crystal potential is altered. Thus, a decrease in resistivity of MSLs in the presence of magnetic field results from reduced crystal potential due to the extra potential introduced by the magnetic field. The reduced potential ensures less amount of scattering, which is the reason why electrons take longer time to return to equilibrium distribution as the magnetic field increases.

Magnetization of metals is a result of spin channel redistribution in magnetic field and it saturates at certain values of the field with no further spin redistribution [12]. Baibich et al. [10] reported saturation field of 20 kG for Fe30Å/Cr9Å₄₀. This suggests a limiting electron incident angle β_s at which further increase in $\mathbf{B}$ no longer alters the direction in which electrons strike at the interface. This is obvious from Fig. 2 in which for $\beta = 90^\circ$ electrons move parallel to interface with no observable resistivity because Eqn. (19) gives: $\rho_{90^\circ} = 0$.

$$\text{Co10Å/Cu10Å}_{15}$$

For this structure every other parameter remains as before except:

Co potentials [13]: $U^\uparrow = -7.43 \text{ eV}$; $U^\downarrow = -5.7 \text{ eV}$.
Cu potentials [2]: $U^{\uparrow,\downarrow} = -8.54 \text{ eV}$.

Anti-parallel relaxation time: $\tau_{AP} = 4.38 \times 10^{-17} \text{ s}$

The chosen value of τ_{AP} gives: $\rho \approx 19.7 \mu\Omega\text{cm}$. Table 2 lists the deduced experimental parallel alignment resistivity $\rho(H)$ and its calculated values. The favourable agreement of both is quite obvious. Fig. 6 illustrates comparable observed and calculated GMR. However, theoretical GMR tends below zero at higher fields; this is but a minor discrepancy born out of approximations and choice of parallel state relaxation times τ_p at higher fields. It is observable from resistivity curve in Fig. 7 that parallel alignment resistivity decreases as τ_p increases, which is typical in magnetoelectronics experiments. And, as mentioned earlier, an increase in τ_p is attributed to a reduced effective crystal

potential due to additional potentials from the magnetic field. It makes the electrons take longer time to return to equilibrium distribution.

Table 2: Magnetoresistance and parallel state resistivity of Co10Å/Cu10Å₁₅.

H(T)	*GMR(%)	Resistivity ($\times 10^{-7}\Omega m$)	
		**Expt.	Theory
0.00	50.00	3.05	2.98
0.05	47.00	2.98	2.92
0.16	39.00	2.82	2.76
0.22	33.30	2.71	2.64
0.27	28.00	2.60	2.54
0.38	21.30	2.46	2.41
0.51	16.00	2.35	2.30
0.54	12.00	2.27	2.22
0.73	6.70	2.17	2.12
0.92	2.70	2.08	2.04
1.03	1.30	2.06	2.01
1.57	0.00	2.03	1.98
2.00	0.00	2.03	1.98
3.00	0.00	2.03	1.98

*From the GMR curve in the relevant literature.

**Deduced from reported *GMR.

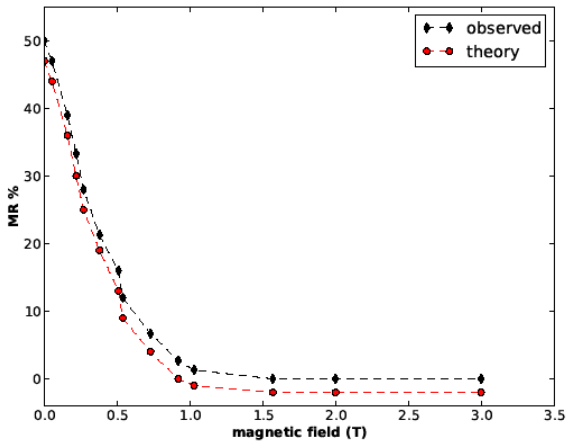


Fig.6: Experimental and theoretical GMR of Co10Å/Cu10Å₁₅ as function of magnetic field. (Experimental values from [11]).

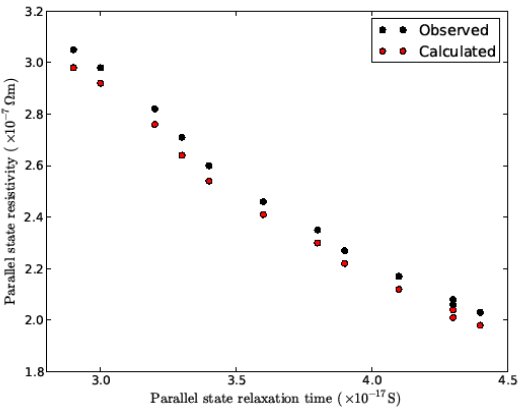


Fig.7: Experimental and theoretical parallel state resistivity of Co10Å/Cu10Å₁₅ as function of parallel state relaxation time. Top curve: experimental values. (Experimental values deduced from [11]).

$Co(t)/Cu(Cr)15\text{\AA}|_6$

As before, other parameters are retained save those that are under-listed. The same relaxation time is used in order to compare results for the involved systems.

- Co thickness: 5 – 25 Å in steps of 5 Å.
- Antiparallel relaxation time, τ_{AP} : $(6.00, 6.30, 6.35, 7.10, 7.44) \times 10^{-14}s$
- Parallel relaxation time, τ_P : $(1.58, 1.47, 1.27, 1.20, 1.11) \times 10^{-13}s$

For the reason of increasing number of atoms and scattering centres as thickness becomes larger, τ_{AP} is chosen to increase with thickness. On the other hand, τ_P reduces due to implied perturbation of incidence angle by **B**. Interesting results of the calculations are illustrated in Figs. 8-13.

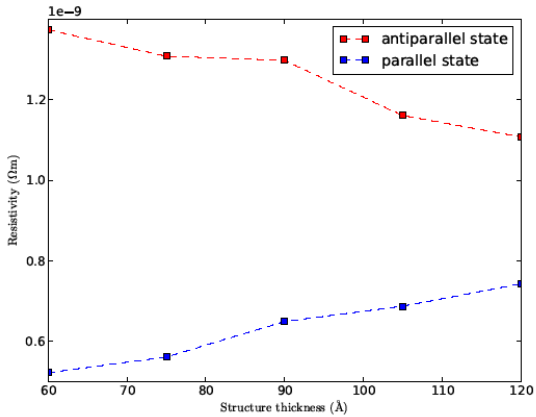


Fig.8: Resistivity of Co/Cr₆ as a function of thickness. Top curve: antiparallel state resistivity.

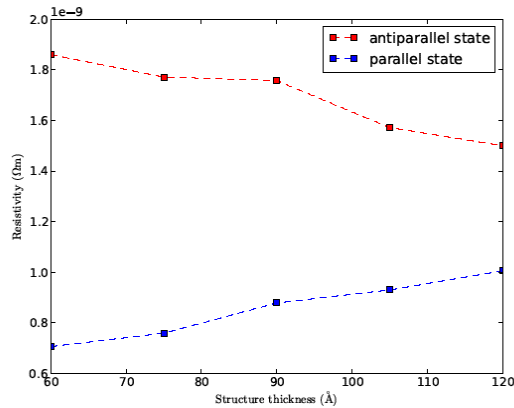


Fig.9: Resistivity of Co/Cu₆ as a function of structure thickness. Top curve: antiparallel state resistivity.

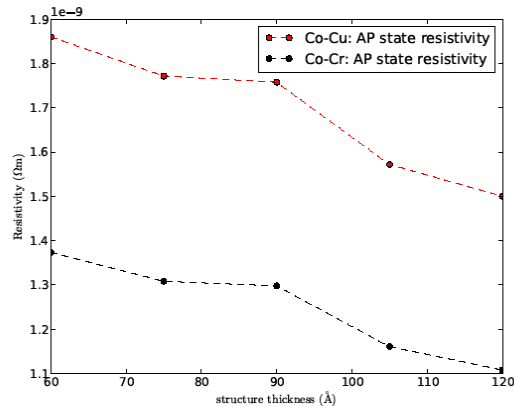


Fig.10: Anti-parallel state resistivities of Co/Cr₆ and Co/Cu₆ as function of structure thickness. Top curve: Co/Cu₆.

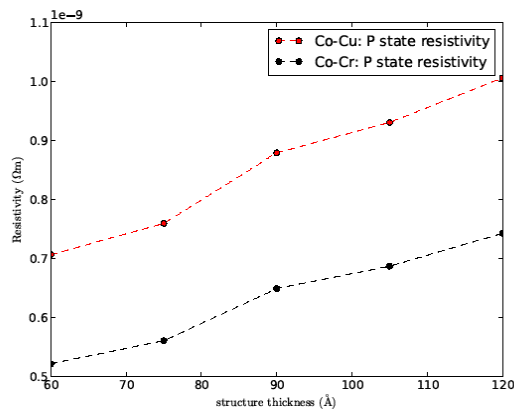


Fig.11: Parallel state resistivities of Co/Cr₆ and Co/Cu₆ as a function of structure thickness. Top curve: Co/Cu₆.

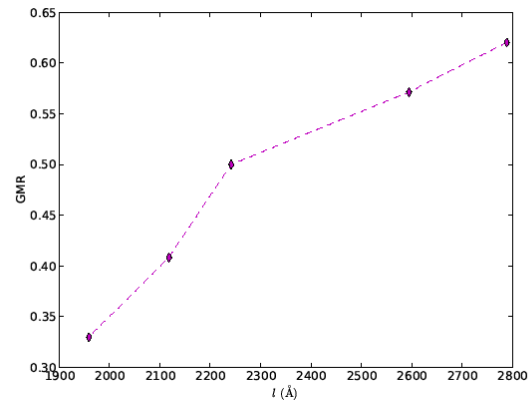


Fig.12: Co/Cr₆: GMR as a function of parallel state mean free path.

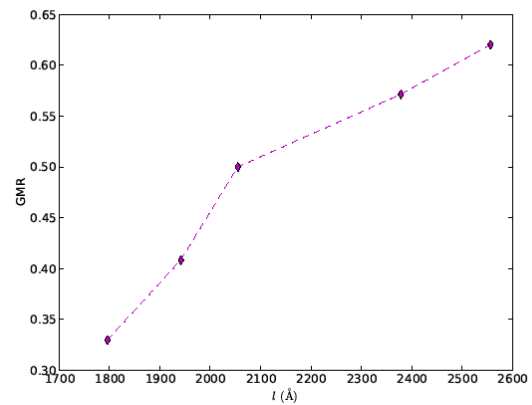


Fig.13: Co/Cu₆: GMR as function of parallel state mean free path.

It is found that AP state resistivities of both systems reduce as thickness of the structure increases and are larger than those of parallel state; the latter however are on the rise with thickness (Figs. 8 and 9). This results to “normal GMR”, where resistivity at parallel state is smaller and which occurs mostly in systems with similar ferromagnetic layers. A comparison of resistivities in Figs. 10 and 11 shows that Co/Cu₆ exhibits higher magnitudes in both antiparallel and parallel states, which demonstrates Co/Cr₆ to be a better conducting and magnetoresistive system. This is buttressed further by electrons having longer trajectory in Co/Cr₆ (Fig. 12) than in Co/Cu₆ (Fig. 13) for the same GMR values. This implies that electrons travel longer before getting scattered in Co/Cr₆. Hence, the mean free path is inversely proportional to total structure potentials, which is

determined, for structures with fixed ferromagnetic layers, by the potentials of the spacer (normal metal) layer.

We stated earlier that changes in resistivity are caused by perturbation from **B**. Therefore, in Figs.8 and 9, the rise of parallel state resistivities with thickness shows that the perturbation is directly proportional to thickness. And, as larger thickness correspond to lower GMR, we conclude that small perturbation, found in thin structures, facilitate large GMR and is the reason GMR occurs in nano scale structures. Conversely, large perturbation suppresses GMR in both thin and thick films.

S-d scattering is determined by the degree of alloying at interfaces and so to some extent it gives a measure of the roughness of interface. In these calculations leading to results presented thus far, we observed that s-d potentials have no noticeable contribution to the GMR. This leaves the bulk scattering as the main mechanism for GMR, a fact that was assumed while we were developing our resistivity model. However, in the case of crystal potentials being uniformly zero and considering non-vanishing s-d potentials, the velocity and Fermi vector (both dependent on total energy) will be small and lead to a small magnitude GMR by virtue of resistivity at **B** being large and close to resistivity in the absence of **B** (cf. Eqn. (19)). Thus interface roughness suppresses GMR.

In Hood and Falicov [2], for instance, roughness of outer surfaces is accounted for via specular factor P between 0 and 1. $P = 1$ denotes complete specular scattering, which makes an electron traverse a ferromagnetic layer twice making a tri-layer equivalent to a superlattice. In practice specular scattering surfaces has been achieved by oxidizing the outer surfaces of a structure [13]. Now, from its development, our model adopts specular scattering surfaces by confining electrons in infinite square well. One then notices, the ease of its application to any number of layers and the favourable account of oxidised outer surfaces.

4. Conclusion

The Drude-like model presented herein reduces the necessary parameters for the characterization of CIP and CPP GMR to only two measurable quantities: the mean free path and relaxation time. In this regard, it substantiates the statement of Miller et al. [4] that the assumption of Drude-like formalism would make GMR a probe of spin-up and spin-down mean free paths. The model shows that external magnetic field perturbs the trajectory

of itinerant electrons and the total structure potentials, causing the electrons to describe a helix as they propagate.

Appendix A

Asymmetry of Fermi vector

A logical implication of spin-dependent bulk potential being a mechanism for GMR is that Fermi vector will be spin polarised. Fig.A1 is a 2-dimensional lattice of metal in which the lattice points are occupied by atoms. The primitive cell is the square of volume a^3 outlined by four atoms where **a** is lattice vector. Free electrons of the four atoms move around within the square in a circle of radius k_F the Fermi vector. The circle, an approximation to the square primitive cell, is an alternative choice for the primitive cell.

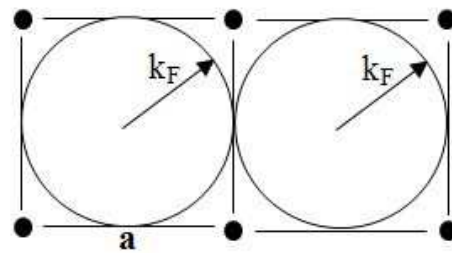


Fig.A1: 2-dimensional lattice with two alternative choices for primitive cell: a square and a Fermi circle. In 3D, the circle is a sphere.

In 3-dimensional lattice, the electrons move in a sphere of volume

$$a^3 \approx \frac{4\pi k_F^3}{3} \quad (A.1)$$

As the reciprocal lattice vector

$$b = \frac{2\pi}{a} \quad (A.2)$$

The volume of reciprocal primitive cell, the Brillouin zone

$$b^3 = \left(\frac{2\pi}{a}\right)^3 \quad (A.3)$$

On account of exclusion principle, possible free electron states allow two opposite spins. Let N be number of spins and n , the total density of electrons. Then,

$$\begin{aligned}
 \frac{N}{b^3} &= n \\
 &= \frac{a^3}{8\pi^3} N \\
 &= \frac{4}{3} \pi k_F^3 \frac{N}{8\pi^3} \quad (A.4)
 \end{aligned}$$

For one spin ($\alpha = \uparrow$ or $\downarrow$), $N=1$, Eqn. (A.4) gives the spin-dependent Fermi vector

$$k_F^3 = 6\pi^2 n_\alpha \quad (A.5)$$

Where, n_α is density of electrons with that spin. It follows from the last result that at Fermi level the resultant Fermi vector

$$\begin{aligned}
 k_F^3 &= \frac{k_F^{\uparrow 3} + k_F^{\downarrow 3}}{2} \\
 &= \frac{6\pi^2}{2} (n^\uparrow + n^\downarrow) \\
 &= 3\pi^2 n \quad (A.6)
 \end{aligned}$$

This is the conventional form and as shown it is really a mean value on account of the exclusion principle. Depending on whether or not the crystal potential is spin dependent, $k_F^\uparrow$ and $k_F^\downarrow$ may or may not have the same magnitude. In ferromagnets with spin polarised potentials, $k_F^\uparrow \neq k_F^\downarrow$.

Eqn. (A.5), and the steps leading to it, established the fact that the spin asymmetry of Fermi vector is an intrinsic property of metals. This is because of the following physical antecedents.

- i. Pauli principle permits two electrons whose magnetic quantum numbers are not equal. Their detailed properties are, in essence, not the same.
- ii. Fermi level is the highest filled band and is a degenerate total energy level for electrons of opposite spins. Individual kinetic and/or potential energies of the spins are not degenerate.
- iii. Resolution of energies of opposite spins (Stoner's criterion) is possible only if they exist *ab initio*. In other words, magnetic field makes the difference explicit.

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