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LETTER TO THE EDITOR

Conductance oscillations in transition metal superlattices

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Abstract. We present a numerical study of conductance oscillations of transition metal multilayers as a function of layer thickness. Using a realistic material-specific tight-binding model, we show that for disorder-free layers with random thicknesses but clean interfaces, long-period oscillations in the conductance can occur, which are reminiscent of those found in structures exhibiting GMR. Using a heuristic effective mass model, we argue that these oscillations arise from beating between the Fermi wavevector and a class of wavevectors characteristic of the superlattice structure.

Oscillations in transport properties of metallic superlattices have been largely studied in magnetic–non-magnetic multilayers, which exhibit giant magnetoresistance (GMR), both from an experimental [1–3], and a theoretical [4–8] point of view.

Recently a new set of measurements on Ni–Co [9–13], multilayers revealed the possibility of long-period oscillations of a different origin, whereas, measurements on Ag–Pd [13], Ag–Au and Ag–Cu [14] multilayers have not shown long-period oscillations. On the one hand, the Ag based multilayers are entirely non-magnetic. On the other, the Ni–Co multilayers were measured in high magnetic field, far above the coercive field of the structure, which rules out magnetic misalignment between magnetic layers as the source of the oscillations. In these experiments, all the measurements were conducted with the current in plane (CIP) configuration and to-date, no measurements have been carried out in the current perpendicular to the planes (CPP) configuration.

In this letter we predict that such oscillating behaviour can also occur with the CPP, in clean superlattices with very good interfaces, but where the layer thickness fluctuates randomly. Moreover this can explain the absence of such oscillations in the experiments on Ag–Pd [13], Ag–Au and Ag–Cu [14]. To the best of our knowledge this is the first time that long-period conductance oscillations in the CPP configuration have been identified in realistic calculations for such systems.

To address this problem, we have developed a very efficient technique to calculate transport properties of a finite multilayer attached to semi-infinite pure crystalline leads, as sketched in figure 1. The technique, which will be discussed in detail elsewhere [15], is very general and can be readily applied to a wide range of GMR multilayers, or TMR spin valves [16, 17]. Our calculations are based on the Landauer–Büttiker formalism [18], using s–p–d tight-binding Hamiltonians with nearest-neighbour hopping, which reproduce

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accurately the band structure of the materials considered [19]. The conductance Γ^σ of a given spin species is obtained from the Landauer formula [18]

$$\Gamma^\sigma = \frac{e^2}{h} T^\sigma \tag{1}$$

where T^σ is the total transmission coefficient for the spin σ ($\sigma = \uparrow, \downarrow$) calculated at the Fermi energy. The latter is obtained by extracting the S matrix from the total Green function G of the superlattice in contact with external leads. The total Green function is calculated via Dyson's equation, starting from the surface Green function g of the leads and an effective Hamiltonian H_{eff} describing the finite multilayer. In all the following calculations we consider a perfect lattice match between clean fcc layers and hence $k_\parallel$ is a good quantum number (the symbol $\parallel$ represents the in-plane coordinates and the symbol $\perp$ the direction of the current perpendicular to the planes). The Hamiltonian is diagonalized in the Bloch basis to yield

$$\Gamma^\sigma = \sum_{k_\parallel} \Gamma^\sigma(k_\parallel) = \frac{e^2}{h} \sum_{k_\parallel} T^\sigma(k_\parallel) \tag{2}$$

where the sum over $k_\parallel$ extends over the two dimensional Brillouin zone. In what follows, we employ of order 10^4 $k_\parallel$-points, which is sufficient to render effects due to the finite number of $k_\parallel$-points negligible compared with the oscillations of interest. In what follows, for Ni–Co and Ag–Pd multilayers, we calculate the total conductance of the two independent spin channels as a function of layer thickness, in the limit that the spin-flip and phase-breaking lengths are infinite. It should be noted that the majority bands of Ni and Co are s–p-like and are closely aligned. On the other hand the minority bands are d-like and possess a relative shift in energy of about 0.7 eV. Hence we expect a large contribution to the conductance from the majority channel and a small contribution from the minority channel. For Ag–Pd the situation is qualitatively different, because at the Fermi energy the DOS of Ag is dominated by s–p electrons, while in Pd it is dominated by d electrons. As a consequence one expects strong interband scattering at the interfaces between the different metals.

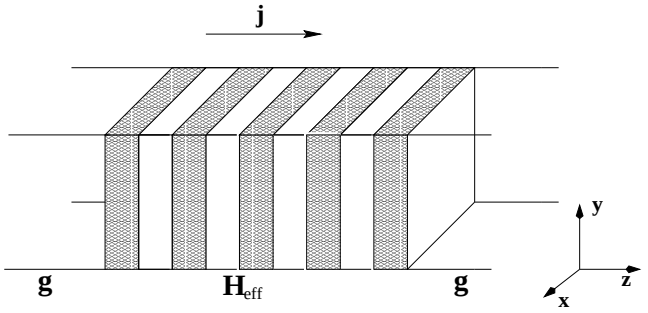

Figure 1. Finite multilayer connected to pure crystalline semi-infinite leads. g are the surface Green functions describing the leads and H_{eff} is the effective Hamiltonian describing the multilayer.

Following reference [5], we consider a pseudorandom layer arrangement, in which a finite A–B multilayer, attached to semi-infinite leads of material A, possesses B-layers of fixed thickness l_B and A-layers of random thicknesses l_A which are allowed to fluctuate by ± 1 atomic plane (AP) around a mean value $\bar{l}_A$ (with equal probability for $\bar{l}_A$, $\bar{l}_A \pm 1$). In all the following simulations, we consider multilayers consisting of 10 A–B bilayers and

for each l_B, show results for the average conductance of 10 random configurations of the A-layers.

For Ni–Co and Ag–Pd respectively, figures 2 and 3 show the mean conductance as a function of l_B, along with error bars for the standard deviation in the mean σ_m. While the latter is smaller than the underlying conductance variation, it should be noted that this is not the case for the standard deviation σ in the distribution of individual conductances, which for an ensemble of m realisations satisfies $\sigma_m \sim \sigma/\sqrt{m}$, where $m = 10$ for figures 2 and 3. For small m, σ is of the order of the conductance fluctuations themselves, thereby masking any underlying trend. In experiments involving a large number n of bilayers, such that the total length $l = n(l_A + l_B)$ is larger than the phase-breaking length l_ϕ (due to incoherent scattering processes), the sample may be viewed as comprising l/l_ϕ samples in series and therefore the total resistance is the sum of l/l_ϕ statistically independent resistances. This suggests that multilayers with large number of bilayers are needed in order to detect reproducible conductance oscillations, as indicated by several experiments [9–13]. The figures suggest the presence of long-period oscillations on a scale greater than the atomic spacing, with amplitudes not exceeding 25% of the mean conductance. Moreover the Ni–Co system shows smaller oscillations than the Ag–Pd system, and despite the fact that the conductance of the majority spin channel is almost double that of the minority, the oscillations arise predominantly from the minority spins, where the scattering is strongest.

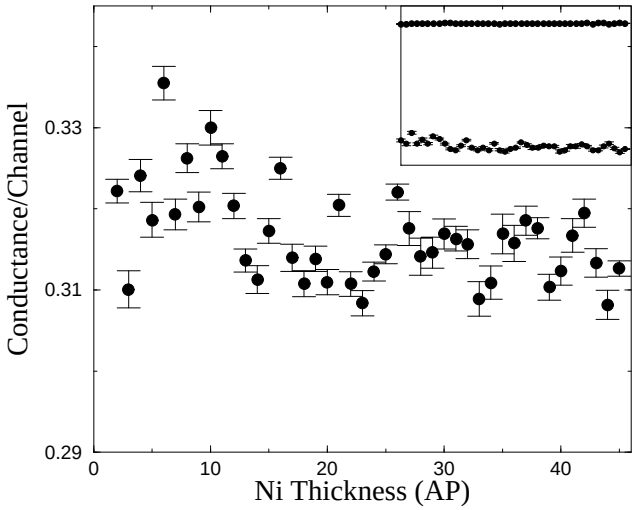

Figure 2. Conductance of Ni–Co multilayers as a function of the Ni thickness. The Co thickness is 10 atomic planes. The inset shows the two spin conductances on the same scale with the upper plot for majority spin and the lower for minority spin. The error bars correspond to the root-mean-square deviation of the mean.

To understand how quantum interference of the conduction electron wave-functions might give rise to long period oscillations, and to check the consistency of the tight-binding calculations, we now develop a heuristic continuum model, within the effective mass approximation, describing an infinite 3D superlattice with a Kronig–Penney potential and a parabolic band. The spin-dependent Hamiltonian for such a system is

$$H^\sigma(\boldsymbol{r}) = -\frac{\hbar^2}{2}\left[\frac{\nabla_{xy}^2}{m^*(z)} + \frac{\partial}{\partial z}\frac{1}{m^*(z)}\frac{\partial}{\partial z}\right] + V^\sigma(z) \tag{3}$$

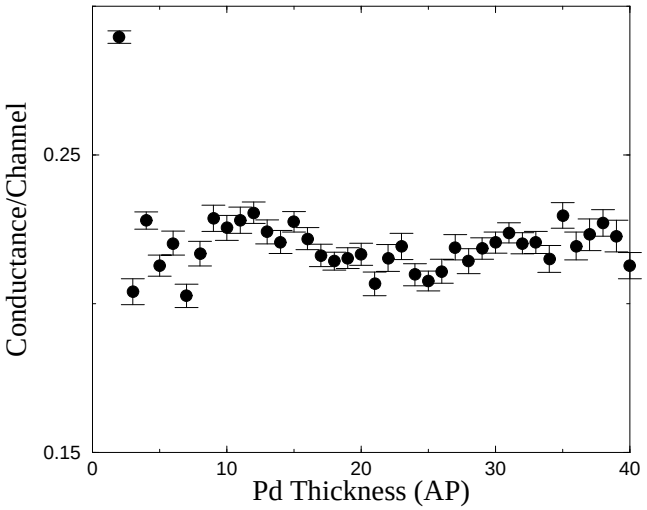

Figure 3. Conductance of Ag–Pd multilayers as a function of the Pd thickness with an average Ag thickness of 5 atomic planes.

where ∇^2_{xy} is the 2D Laplacian. Since the structure of figure 1 possesses translational invariance in the x–y directions, the spin-dependent Kronig–Penney potential $V^\sigma(z)$ and the effective mass $m^*(z)$ are functions of z only. Consequently the problem can be mapped onto a $k_\parallel$-dependent 1D problem, whose Hamiltonian is

$$H^\sigma(z;k_\parallel) = -\frac{\hbar^2}{2}\frac{\mathrm{d}}{\mathrm{d}z}\frac{1}{m^*(z)}\frac{\mathrm{d}}{\mathrm{d}z} + \frac{\hbar^2 k_\parallel^2}{2m^*(z)} + V^\sigma(z). \tag{4}$$

For each $k_\parallel$ and spin σ, an eigenstate at the Fermi energy contributes e^2/h to the conductance of this infinite periodic structure. In the general case, the eigenstates can be obtained numerically using standard transfer matrix techniques. First consider the case of constant $m^*(z)$, where the problem can be solved analytically. Since the Hamiltonian (4) depends on $k_\parallel$ only through an energy shift, one finds that the conductance per unit area has the simple form

$$\Gamma = \frac{8\pi e^2 m^*}{h^3}\Delta = \frac{8\pi e^2 m^*}{h^3}\sum_n \Delta_n \tag{5}$$

where Δ_n is the bandwidth of the nth energy band of the Hamiltonian

$$H^\sigma(z) = -\frac{\hbar^2}{2m^*}\frac{\mathrm{d}^2}{\mathrm{d}z^2} + V^\sigma(z) \tag{6}$$

and the sum is over all occupied minibands. The form (5) assumes an infinite cross section (constant DOS in the transverse direction), which is a good approximation to the finite cross sections considered (~ 200 Å $\times$ 200 Å). Consider an infinite superlattice composed of materials A and B, with layer-thicknesses l_A and l_B ($l_\mathrm{A} + l_\mathrm{B} = L$), and Kronig–Penney potential $V = V_o$ ($E_\mathrm{F} > V_o$) in the metal A and $V = 0$ in the metal B. If $k_\perp$ is the Bloch vector in the direction of the current, the secular equation is

$$\cos(k_\perp L) = \cos(k_\mathrm{A} l_\mathrm{A} + k_\mathrm{B} l_\mathrm{B}) - \frac{(k_\mathrm{A} + k_\mathrm{B})^2}{k_\mathrm{A} k_\mathrm{B}}\sin(k_\mathrm{A} l_\mathrm{A})\sin(k_\mathrm{B} l_\mathrm{B}) \tag{7}$$

with $k_{\mathrm{A}}(E) = \sqrt{2m^*(E - V_o)}/\hbar$ and $k_{\mathrm{B}}(E) = \sqrt{2m^*E}/\hbar$. Based on this expression, we now argue that the bandwidths exhibit several periods of oscillation as the layer thicknesses are varied.

To describe Ni–Co multilayers, we vary the thickness of metal B keeping the thickness of metal A fixed. To understand the oscillatory behaviour of the bandwidths, we note that equation (7) cannot be satisfied at energies for which

$$k_{\mathrm{A}}(E)l_{\mathrm{A}} + k_{\mathrm{B}}(E)l_{\mathrm{B}} = m\pi \tag{8}$$

where m is an integer. Hence at $E = E_F$ and fixed l_A, successive bandgaps appear at the Fermi energy E_F when l_{B} changes by

$$l_{\mathrm{B}}^m = \frac{\pi}{k_{\mathrm{B}}(E_{\mathrm{F}})}m = \frac{\pi\hbar}{\sqrt{2m^*E_{\mathrm{F}}}}m = l_{\mathrm{B}}^{\mathrm{F}}m. \tag{9}$$

Equation (9) introduces the first period of oscillation $l_{\mathrm{B}}^{\mathrm{F}}$. The second period corresponds to the presence of narrow gaps below the Fermi energy. From equations (7) and (8) narrow bandgaps appear at the energies

$$E_A^{(n)} = \frac{\hbar^2\pi^2n^2}{2m^*l_{\mathrm{A}}^2} + V_o \tag{10}$$

whenever the lengths l_{B} equal

$$l_{\mathrm{B}}^{(n)} = \frac{\pi\hbar}{\sqrt{2m^*E_A^{(n)}}}. \tag{11}$$

The total bandwidth Δ and hence the conductance per unit of area (5) are oscillating functions with periods $l_{\mathrm{B}}^{\mathrm{F}}$ and the $l_{\mathrm{B}}^{(n)}$. All these periods are of order λ_F (i.e. few Å), but beating between them can give rise to long-period oscillations. It is important to note that the Fermi period is defined only through the Fermi energy, while the periods $l_{\mathrm{B}}^{(n)}$ depend critically on the superlattice geometry. In particular, because the energies corresponding to periods (10) depend on $1/l_{\mathrm{A}}^2$ and must not exceed the Fermi energy, the number of $l_{\mathrm{B}}^{(n)}$ depends on the thickness of the metal A. If l_{A} is large, a large number of $l_{\mathrm{B}}^{(n)}$ periods will be present and the beating pattern will be complex. On the other hand, if l_{A} is small, few $l_{\mathrm{B}}^{(n)}$ will be present, giving rise to a simple beating pattern. A numerical evaluation of equation (5) is shown in figure 4. For the chosen parameter in this plot, we expect only one $l_{\mathrm{B}}^{(n)}$ and clear beats are observed, with period $2l_{\mathrm{B}}^{(1)}l_{\mathrm{B}}^{\mathrm{F}}/(l_{\mathrm{B}}^{(1)} - l_{\mathrm{B}}^{\mathrm{F}})$. Since the $l_{\mathrm{B}}^{(n)}$ periods are characteristic of the superlattice structure we predict that the period of the long oscillations can be set by choosing the appropriate superlattice geometry. Of course in a real superlattice, the B-metal thickness can only be changed in units of the interatomic spacing. The solid dots in figure 4 highlight the conductances associated with such a discrete set of thicknesses.

The above dependence of oscillations on the multilayer structure is missed by a trilayer quantum well approach to conductance oscillations and GMR [20], where only two periods have been identified. The first of these p^{FS} depends on the extremal Fermi surface radius of the spacer forming the well, and in the parabolic band approximation corresponds exactly to the period $l_{\mathrm{B}}^{\mathrm{F}}$. The second period p^{cp} depends on the cut-off of the sum over the $k_\parallel$ and in the parabolic approximation, on the energy difference between the Fermi energy and the step potential V_o. In our superlattice description, this period is replaced by the class of periods $l_{\mathrm{B}}^{(n)}$, which are a function of the superlattice structure itself. This structural dependence of the oscillation periods is the key to understanding the apparent non-reproducibility of the long period oscillations from sample to sample, observed in some of the experiments

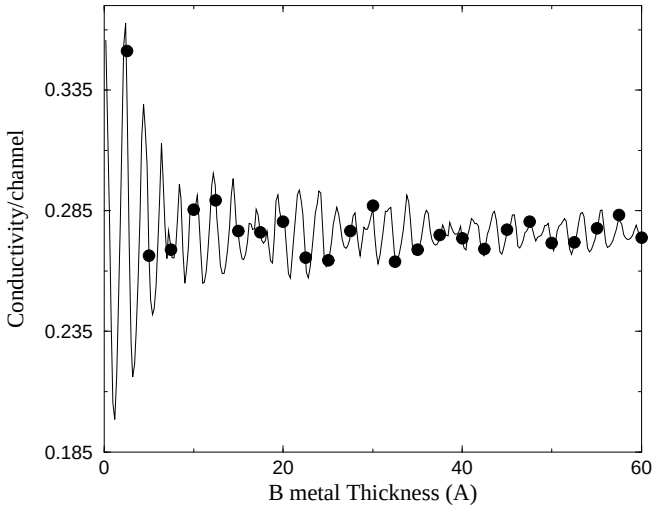

Figure 4. Conductivity per channel in the effective mass approximation. The parameters are $E_{\mathrm{F}} = 10$ eV, $V_o = 6$ eV, $m^* = 0.5$ MeV, $l_{\mathrm{A}} = 8$ Å.

[14]. For those cases where we expect the mass to be significantly different in the two materials (e.g. mainly s–p-like in one material and mainly d-like in the other) we have shown that the Kronig–Penney model reproduces the main features of the more accurate tight-binding model, with physically reasonable choices of the band offsets and effective masses. Furthermore figures 2 and 3 demonstrate that these beating features are preserved when a more realistic material-dependent effective mass is used.

Bearing in mind that our analysis describes the CPP configuration, we can also speculate on the absence of the oscillations in other recent experiments [14, 13]. Ag–Cu [14] exhibits very good phase separation between the different metals and hence it should be a good candidate for observing conductance oscillations. However the band match between Ag and Cu is very good, resulting in a very small scattering potential at the interface. In the effective mass approach this means a very small step potential V_o with respect to the Fermi energy. A large number of periods $l_{\mathrm{B}}^{(n)}$ will be present and the beats will be difficult to detect. The same argument is valid for Ag–Au [14]. In addition the high miscibility of Ag and Au results in dirty interfaces. Ag–Pd [13] is in theory a good candidate to show conductance oscillations because of the large mismatch between the Ag and Pd bands. Unfortunately interdiffusion at the interface is difficult to avoid and the elastic mean free path will be quite short. Finally, we observe that for Ni–Co [9–12, 14], the majority band reproduces roughly the situation of Ag–Cu, while the scattering in the minority band is quite large. According to the effective mass model the minority band will possess a low conductance with large oscillations, while the conductance of the majority band will be large and the oscillations small. This is precisely what we obtain from the material-specific tight-binding calculations. The absence of oscillations found in [14] for Ni–Co multilayers may be due to the diffusive nature of the multilayers. In fact in such experiments the resistances involved are about five times larger than the ones of [9–12], and the mean free path is much shorter. This suggests that the transport is not only non-ballistic, but also that the absolute error in the resistance measurements may become comparable to the observed magnitude of the oscillations.

In summary, we have investigated the possibility of large amplitude long-period oscillations in metallic superlattices in the ballistic regime. Accurate tight-binding calculations with the current perpendicular to the plane and superlattices with pseudorandom layer thicknesses, suggest the possibility of such oscillations. An effective mass analysis provides a qualitative understanding of the nature of the oscillations and highlights their dependence on the superlattice geometry. We have shown that an infinite multilayer differs significantly from a trilayer. In the latter the oscillations depend only on the band structure of the materials, while in the former there is also a dependence on the multilayer geometry. The number of the characteristic oscillation periods is different in the two cases, because the trilayer oscillations depend only on the Fermi surface, while in a superlattice these depend also on the superlattice period.

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