A Superlattice Effect in the Resistivity of Multilayers

Tat-Sang Choy, Jian Chen, and Selman Hershfield
Department of Physics and National High Magnetic Field Laboratory,
University of Florida, 215 Williamson Hall, Gainesville, FL 32611

Abstract—**Calculations are presented of a superlattice effect, observable in samples where most of the scattering is at sharp interfaces. As the layer thicknesses change, oscillations in the resistivity of up to 100% are found. These oscillations are due to interface disorder breaking the degeneracy of certain states, causing them to have nodes at the interfaces. The states with nodes have high conductivities, leading to a "short-circuit" effect. Only for special thicknesses is it possible for a state to have nodes at all the interfaces. Hence, the oscillations occur as a function of layer thickness. Spreading the width of the interfaces or increasing the ratio of bulk disorder to interface disorder reduces the effect.**

I. Introduction

Although magnetic multilayers are superlattices, there is little evidence for coherent superlattice effects in the conductivity or resistivity of multilayers. This is to be contrasted with semiconductor heterostructures where there is clear evidence for minibands. The origin of this difference is presumably the smaller wavelengths and larger disorder in magnetic multilayers. In this paper we present calculations of a superlattice effect which can exist in the presence of large interface scattering so long as the bulk disorder is small and the interfaces are sharp. This effect does not rely on the formation of minibands, but rather on some states scattering more weakly off the disordered potential than others.

II. Model

The model we consider is a tight binding hamiltonian

$$H = \sum_{<ij>} t_{ij} c_i^\dagger c_j + \sum_i U_i c_i^\dagger c_i, \qquad (1)$$

where the t_{ij} are the hopping matrix elements between different atoms or orbitals, and the U_i are the diagonal part of the energy. To illustrate the effect we are interested in we use a simple one band model of a two-component superlattice with planes perpendicular to the z-direction. The atoms are on a square lattice with the hopping matrix elements taken to be the unit of energy, $t_{ij} = t = 1$. The on-site diagonal energies for the two materials are chosen to be 2.02 for metal A and 1.78 for metal B in order to mimic materials with similar band structure. The Fermi energy is set equal to zero. Note that this is not a realistic band structure; however, we believe one would see a similar effect if one used the realistic band structure with more bands and the correct parameters in (1) [1], [2].

The disorder is introduced via the impurity averaged Green's function approach within the self-consistent Born approximation [3]. Within this approach the disorder is modeled via fluctuations in the on-site potential, U_i. The mean square fluctuations in the U_i are equal to $\langle \delta U_i \delta U_j \rangle = \delta_{ij} v_i$. We assume that the mean square fluctuations are the same within each layer, i.e., v is a function of z only. The self-energy $\Sigma^{(r)}$ for the retarded Green's function is then local and only depends on z. The retarded Green's function, $G^{(r)}(k_x, k_y, \omega)$, is a matrix in the z positions. It depends on the in-plane wavevectors and the energy. When indices z, z' are given, we are referring to the matrix elements. The two equations for the retarded Green's function and the self-energy are solved self-consistently:

$$\Sigma^{(r)}_{z,z}(\omega) = v(z) \int \frac{dk_x dk_y}{(2\pi)^2} G^{(r)}_{z,z}(k_x, k_y, \omega), \qquad (2)$$

$$G^{(r)}(k_x, k_y, \omega) = [\omega - (H_\perp - 2t\cos k_x - 2t \cos k_y) - \Sigma^{(r)}(\omega)]^{-1}. \qquad (3)$$

In (3) ω is the energy, which will be set equal to the Fermi energy, and $H_\perp$ is the z–dependent part of the hamiltonian which is tridiagonal. Self-consistency guarantees that this approximation is current conserving. Furthermore, the effects described here are not apparent until one has solved self-consistently for the self-energy. After solving for the Green's function, the conductivity is computed via the Kubo formula [3]–[10]. For this self-energy the vertex corrections are identically zero in the CIP geometry. In obtaining a numerical value for the resistivity a lattice spacing of 3.5Å is used for both materials.

III. Results

We present results for a series of samples with a fixed layer thickness for one metal (A) and a variable thickness for the other metal (B). The disorder, $v(z)$, within each layer is set equal to v_{bulk}, while in one of the monolayers at each interface a different value, $v(z) = v_s$ is assigned. As shown in Fig. 1, the resistivity oscillates with the thickness of layer B, t_B, for an A_5/B_{t_B} superlattice. The

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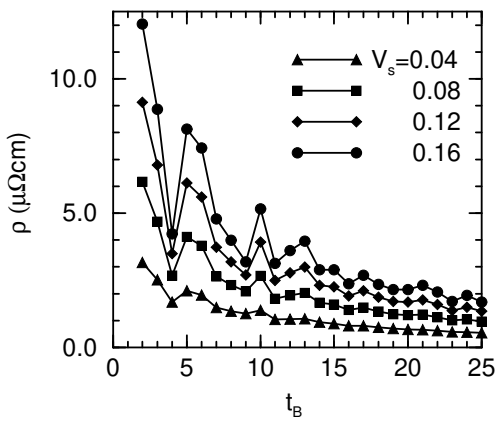

Fig. 1. Effect of surface scattering on the oscillations in superlattices of the form A_5/B_{t_B}. The thickness is in the unit of atomic spacing. The size of oscillations increases as surface disorder v_s increases. The bulk disorder v_{bulk} is fixed at 0.0001.

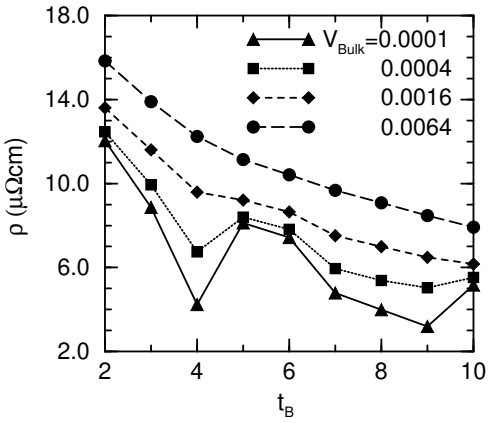

Fig. 2. Effect of bulk scattering on the oscillations in superlattices of the form $A_5B_{t_B}$. The size of the oscillations decreases as bulk disorder v_{Bulk} increases. v_s is fixed at 0.16.

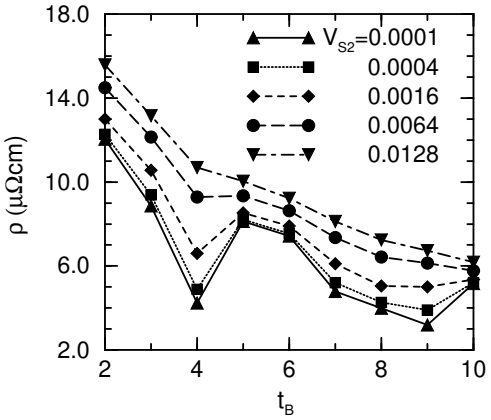

Fig. 3. Effect of spreading the interface on the oscillations again for superlattices of the form $A_5B_{t_B}$. v_{s_2} is the disorder of the monolayer next to the interface. Oscillations are washed out as v_{s_2} increases. v_s and v_{bulk} are fixed at 0.0001 and 0.16, respectively.

strength of the oscillations increases as the surface disorder, v_s, increases. For these parameters, the ratio, v_s/v_{bulk} needs to be about 400 for the oscillations to be clearly observed. With interfaces every 5 lattice spacings, the contribution to the resistivity from interface scattering is about 8 $\mu\Omega cm$ for $v_s = 0.16$ and 2 $\mu\Omega cm$ for $v_s = 0.04$. By contrast the contribution to the resistivity due to bulk scattering is only 0.03 $\mu\Omega cm$ for the $v_{bulk} = 0.0001$ used in Fig. 1. When v_s/v_{bulk} becomes 1600, the size of the oscillations can be as large as 100%.

If instead of increasing the surface scattering, one increases the bulk disorder, the oscillations are washed out. This is demonstrated in Fig. 2, where the resistivity oscillations in A_5/B_{t_B} superlattices are reduced as the bulk disorder increases. Note that it is reasonable for the surface scattering to be large compared to the bulk scattering, but it is not obvious if this large a ratio is realistic. Also, earlier calculations have seen various quantum oscillations in the GMR, and it is not clear whether these are related to the effects seen here [6], [7], [11].

If we fix the ratio of v_s to v_{bulk} while increasing both values, the peak-to-valley ratio of the oscillations remain roughly constant. This indicates that the parameter (v_s/v_{bulk}) is important for determining the size of the oscillations.

We have also performed calculations on the effect of randomizing the layer thicknesses. Random layer thicknesses with a standard deviation ranging from of one to a few Å are introduced. The oscillations in the resistivity are destroyed when the variation is only about one to two Å.

A similar effect can be seen by spreading the interfaces. To study this, we gradually increase the disorder v_{s_2} of a second monolayer next to each interface. As shown in Fig. 3 this has the effect of increasing the width of interfaces. The resistivity oscillations are reduced as we increase v_{s_2}.

We should also stress that this effect is a superlattice effect because it goes away when we reduce the number of bilayers. The mean free path in our calculations ranges from 200 to 500Å, which is at least several times the A/B repeat unit.

IV. Physical Interpretation

To understand the origin of this effect it is useful to examine the eigenvectors of the inverse of the Green's function $[G^{(r)}(k_x, k_y, \omega)]^{-1}$ of (3). The eigenvectors $\psi(z)$ of $[G^{(r)}]^{-1}$ do not depend on k_x and k_y because they only shift the eigenvalues. The $\psi(z)$ enter directly into the computation of the conductivity; however, they are not the eigenvectors of the hamiltonian H. Rather, these functions contain information on how states are scattered from the disordered potential.

The spatial dependence of $|\psi(z)|$ is non-uniform. For most of the eigenstates, $|\psi(z)|$ for z at the interface is non-zero, causing large scattering rates. Therefore, these states have a small contribution to the conductivity. There are some states where $|\psi(z)|$ is small at all interfaces. An example of such a state is plotted in Fig. 4. These states are scattered primarily by the much weaker bulk disorder, and hence have a much larger contribution to the conductivities. When the surface disorder is much

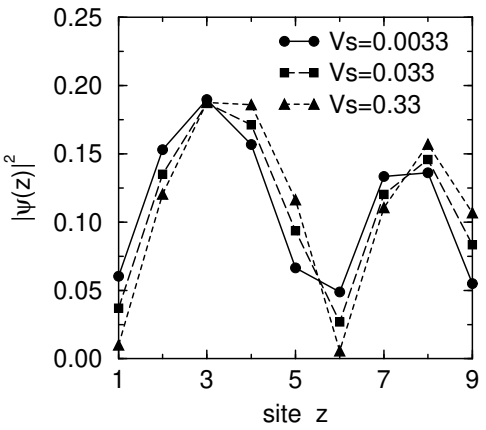

Fig. 4. The magnitude squared of the eigenvectors of $[G^{(r)}]^{-1}$ for a state with a node at the interface. Interface disorder (at $z = 1$ and 6) redistributes the density of this state, effectively creating nodes at these interfaces. The interface disorder v_s varies from 0.0033, when there is no node, to 0.33, when nodes are developed at the interfaces. v_{bulk} is fixed at 0.0001.

larger than the bulk disorder, these special states carry most of the current. However, these states occur only at certain thicknesses, where it is possible to have nodes at all the interfaces, e.g. t_B=4 and 9 in Fig. 1. At other thicknesses, they do not occur and thus the resistivity is higher.

Interestingly enough, the existence of nodes at the interfaces for the above states depends crucially on the interface disorder. For a uniformly disordered sample of one material, $|\psi(z)|$ would be uniform, i.e., have no spatial dependence. In our superlattices, both the periodic potential, U_i, and the disorder break this uniformity. For large disorder at the interface the disorder is actually more important than the periodic potential. The presence of nodes at the interfaces is not a coincidence, but actually a consequence of the usual bonding/anti-bonding phenomena when degeneracies are broken.

V. Relevance to Experiments

We had originally thought that these results were related to the experiments by Gallego *et. al.* in which oscillations in the resistivity are observed in MBE-grown Co/Ni and Ni/Cu superlattices but not in the case of Pd/Ag [12]. The amplitudes of such oscillations have the same order of magnitude as in our calculations. The trend of decreasing amplitudes in the series can also be explained by our model in terms of the decreasing of interface sharpness, which is indeed shown by the sample characterization in the experiments. We also see an increase in the size of the oscillations as the the interface disorder is increased or the bulk disorder is decreased. However, our calculations show that thickness variations tend to destroy the oscillations, which is in disagreement with the experiments.

Furthermore, although temperature dependence is not included in our calculations, if we treat bulk phonon scattering by increasing v_{bulk}, the oscillations are reduced as the temperature is increased. In the experiments by Gallego *et. al.* the oscillations remain roughly the same for a wide range in temperatures from 4 to 300K [13]. Thus, our calculations are unlikely to be an explanation of these experiments and other explanations are necessary [14], [15].

VI. Conclusions

In this paper we have shown that even in the presence of large surface scattering it is possible to see a superlattice effect. The origin of the oscillations in the resistivity is the periodic nature of the disordered interface scattering. For certain layer thicknesses there is a "short-circuit" effect where some states scatter weakly from the disorder at the interfaces. This oscillatory behavior still exists for different choices of Fermi energy and on-site energies. It does not require magnetism; however, it could exist in magnetic materials such as Ni and Co. It does not appear that these oscillations have been seen. In order to observe them one must have very sharp disordered interfaces and surface scattering which is much larger than the bulk scattering.

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