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CONTRIBUTION TO THIN FILM MAGNETORESISTANCE*

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Some aspects of theoretical approaches to the magnetoresistance description are reviewed. The conclusions and illustrative remarks are of tutorial character. The role of magnetic field applied to samples is discussed. The density functional technique is considered in the context of its application to the giant and colossal magnetoresistance when the magnetic field is included.

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1 Introduction

The discovery of the giant and colossal magnetoresistance is one of the most important experimental facts in physics of magnetic materials in the last decade. It is interesting for many aspects, first of all, for their prospective applications in different areas of technology, but also, it brings a new light in the case of fundamental studies of nanoscale objects.

The giant magnetoresistance originally observed in magnetic multilayers [1] is a decrease of the electrical resistance due to the ferromagnetic alignment of magnetic layers (e.g. Fe, Co) separated by a nonmagnetic spacer layer (e.g. Cr, Cu, Ag) caused by an external magnetic field with respect to the resistance corresponding to the zero field when the magnetic layers exhibit antiparellel alignment.

The colossal magnetoresistance was found first in epitaxial lanthanium manganite thin films which are of the perovskite-like oxides structure [2]. The colossal magnetoresistance behaviour seems to be connected with the electronic processes in the elementary cells of the perovskite-like geometry. The effect is very sensitive to lattice parameters and, first of all, to the ratio of numbers of cations which occupy the proper site positions and change their valence due to the electronic transfer. (e.g. Mn^{3+}/Mn^{4+}). Thus, the structure plays an important role in the description of the colossal magnetoresistance which appears when the cations of different valence alternate in the crystal lattice sites.

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The most effective mechanism responsible for the magnetoresistance is the spin-dependent scattering of the conduction electrons at the interfaces in the case of the multilayers [3] as well as the active centres in the dispersive samples [4]. In particular, the granular structures correspond to the conditions in which the grain boundaries spin dependent scattering is evident.

At present, the most suitable approach to the magnetoresistance description seems to be the model introduced by Hood and Falicov [5] and based on Camley and Barnaś [3] description for giant magnetoresistance in multilayers. In the present contribution the model is taken into account as a reference for the discussion of some methodological questions which seem to be of great importance for the magnetoresistance behaviour. The scattering conditions are modified now by the applied magnetic field which also influences the magnetic ordering configurations.

2 The role of the applied magnetic field

The model of Hood and Falicov [5] is an extension of the Fuchs-Sondheimer theory of the free conduction electron transport in thin films [6] where the distribution of electrons is given by the Boltzmann equation for a sample taken in the form of a threelayer composed of two ferromagnetic covers and a non-magnetic spacer. The ferromagnetic layers are described by the band model of itinerant electrons embedded into metal spin dependent potentials which are responsible for different densities of states for the two different orientations of spins. The electrical current is a sum of the currents in two independent channels for electrons with oriented spins. The basic model is developed in many aspects. In particular, the interfacial scattering conditions are considered [7] and the interaction between two spin-dependent channels is taken into account [8].

The model predicts the dependence of the magnetoresistance on the thickness of the magnetic and nonmagnetic spacer layers in the case of various characterisations for the quality of samples, in particular, for the roughness of their interfaces and surfaces. However, the wide applications of the model do not take into account the description of the magnetoresistance behaviour in the applied magnetic field. Moreover, in the case of the Hood and Falicov model [5] the magnetic field term has been dropped from the Boltzmann equation. Independently of the argument that this term gives an effect which is orders of magnitude smaller than the change of magnetoresistance due to the change of magnetic moment configurations in two outside magnetic layers we would like to notice the methodological aspect of the question.

The semi-classical approach to the Fuchs-Sondheimer theory is based on the equation of motion which is usually substituted to the Boltzmann equation in its classical form. In the considered case the equation of motion contains the Lorentz force whose two terms correspond to the electric and magnetic field contributions. The magnetoresistance depends then on the applied magnetic field due to the magnetic component of the Lorentz force. In particular, the fact is evident in the classical treatment [9] when the magnetoresistance depends on the magnetic field in the case of nonmagnetic samples. We also mention the obvious fact that the applied field and the internal field produced by magnetic band electrons influence conduction electrons in different ways.

When the magnetic field term is neglected in the Boltzmann equation the symmetry of its solution is changed as compared with the situations where the magnetic field term is included. This means that not only the Boltzmann distribution does not depend on the magnetic field but, first of all, the terms of cylindrical symmetry disappear in the Boltzmann function. In contrast, when we keep those terms, the Boltzmann distribution leads via the boundary conditions to the modification of the magnetoresistance. The influence of boundaries modified in such a way seems to be sufficiently strong in accordance to the experimental statements that the electron scattering at the surfaces is more important than inside a sample.

Theoretical investigations of the magnetoresistance have been carried out for multilayers by means of both the quasi-classical Boltzmann approach $[5, 6]$ and the quantum Kubo formalism $[10]$. There is a common opinion that the quasi-classical and quantum approaches are basically equivalent, at least for the case of multilayers. However, the problem seems to us not so clear. Therefore, we present the following remarks.

Both the models are really equivalent when one assumes that the electrons are described in terms of a free quasi-particle model and the Lorentz force perturbes only their movement. In this case the statistical operator appearing in the Kubo formalism and the Boltzmann distribution give equivalent results for the resistance calculated by means of the perturbation theory. But, shortly speaking, the assumption is justified only in the case when the magnetic field term is not taken into account.

However, the considered situations are not equivalent in the classical and quantum case when the magnetic field term is not dropped, even if its contribution is infinitezimally small. The problem is of qualitative nature $[cf.11]$.

The classical and semi-classical Boltzmann approaches in the presence of magnetic field lead to the results which are really equivalent to those discussed in the free quasi-electron models, while the quantum approach gives the description in terms of the Landau levels which are then perturbed by the Lorentz force. Thus, the three-dimensional motion of quasi electrons is replaced by the two-dimensional quantum oscillator states in the plane perpendicular to the magnetic field direction and the one-dimensional motion parallel to the field, which is of a free quasi-particle character.

The applied magnetic field causes, in fact, the reorientation of the magnetization from antiparallel to parallel alignment leading by this rearrangement to the characteristic configurations determining the giant magnetoresistance effect. In the light of the present methodological considerations we can conclude that the magnetic field plays, however, a more important role in the description of the magnetoresistance properties and it cannot be droped from the model for physical reasons. The models, like the Hood and Falicov model, describe only the asymptotic situations.

3 Spin dependent charge distribution

For thin films the conduction electron transport behaviour is influenced by the shape of a sample. The boundary conditions at the surfaces lead to the electric charge distribution across a film $[e.g.12]$. ¿From the physical point of view the charge density is also distributed due to the surface changes of the order-disorder parameter [13] in the case of heterogeneous alloys or multilayers as well as to the proximity effects.

The recent theoretical approaches to the giant megnetoresistance description in layered systems are based on the Kubo formalism with realistic first principle band structure calculations which are developed where the layer Korriga-Kohn-Rostoker method and local density approximation are used to calculate the electronic structure of the mixed slabs $[10]$. The exact quantum mechanical methods incorporate the wave functions for the Boltzmann equation [14] or the tight-binding parametrization of s, p and d bands in order to evaluate the Kubo formula.

The giant magnetoresistance is confined not only to multilayered systems but it is also found in magnetic granular systems in which the ferromagnetic grains are embedded in nonmagnetic environment [4]. In this case clusters are primary models for theoretical considerations of the giant magnetoresistance dependence on the grain sizes with respect to the applied magnetic field which influences the local magnetization vectors distribution. The density functional theory seems to be then the most suitable method which offers the best ab-initio treatment especially via nonlocal generalized gradient approximation approach to exchange and correlation effects [15]. It also provides another impact for better understanding the nature of the interactions between a nonmagnetic atom and the adjacent atoms with partially filled d orbitals at the local molecular level by viewing the bonding-antibonding properties of the molecular wave functions at the cluster Fermi level.

The local density of states obtained by this technique is also the main key in our approach for further calculations of the magnetoresistance. As mentioned at the beginning of the paper the colossal magnetoresistance observed in perovskite-like structures of lanthanium manganites is inevitably connected with the electron transfer between Mn^{3+} and Mn^{4+} ions caused by a partial substitution of La^{3+} ions by doubly charged Ca, Ba or Sr ions. The customary band representation is inappropriate for the description of this charge transfer and the above mentioned cluster method along with its high level treatment of exchange and correlation effects as well as with its use of localized atomic orbitals naturaly comes into consideration. The electronic structure is then a composition of the cluster density of states which can be treated as a periodic unit of the structure. In this way the Fourier transforms of the local density of states can be introduced. The electric current is then calculated at the level of the charge density Fourier components whose statistical distribution is given by the Boltzmann function Fourier component or the statistical operator matrix elements in the Fourier components representation where it is diagonal. While this method is natural for granular systems it is still general enough to provide a common theoretical tool for the study of both the colossal (perovskite structures) and the giant (multilayers) magnetoresistances by a functional definition of the basic unit.

4 Conclusions

The present considerations are general enough to be applied for both the giant and the colossal magnetoresistance description. Moreover, they can also serve for the explanation of the resistance dependence on the applied magnetic field in the case of nonmagnetic samples. In particular, the method describes then magnetoresistance behaviour in non-magnetic alloys, (e.g. $Pd_{1-x}Ag_x$) in agreement with the experimental results [16].

The advantage of the method based on the density functional technique for the giant and colossal magnetoresistances description consists in the presence of the applied magnetic field . From the methodological point of view the present discussion allows us to maintain the conclusion following from general ideas of the quantum field theory. We would like to emphasise that the magnetic field dependence appearing in the wave function phase factor contributes to the density interference term in the case of multi-electronic systems. This does not appear in the classical case when the electronic motion is represented by one particle picture. Thus, the density functional technique is a proper way to account for the quantum nature of the phenomenon.

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