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LETTER TO THE EDITOR

Monte Carlo simulation of colossal magnetoresistance in doped manganese perovskites

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Abstract

Resistance as a function of temperature and applied magnetic field for doped manganese perovskites is simulated on the basis of a random-resistor-network model. The network, consisting of ferromagnetic metallic particles with number density p and paramagnetic insulating particles with number density $1 - p$, is generated through the Monte Carlo method. Approximating p by the reduced magnetization (m) determined from the mean-field theory, we show that the simulation can yield the main features of the colossal magnetoresistance in doped manganese perovskites. Comparisons between simulated and experimental data are also presented for $(La_{1-x}Y_x)_{2/3}Ca_{1/3}MnO_3$ ($x = 0.2$). The excellent agreement between the simulations and experiments gives strong support to the present approach.

Aside from their technological potential, doped manganese perovskites of the form $Re_{1-x}B_xMnO_3$ (Re = rare-earth cation, B = alkaline-earth cation) are important due to the unusual magnetic and electronic properties [1]. Most notable of these properties is the so-called colossal magnetoresistance (MR) [2], a substantial reduction of resistivity caused by the applied magnetic fields. For the optimal cases in which $x \sim 1/3$ and the tolerance factor $t \geqslant 0.91$, the compound undergoes a transition from high-temperature insulating behaviour to low-temperature metallic behaviour. This electronic transition is accompanied by a simultaneous paramagnetic (PM)-to-ferromagnetic (FM) transition at almost the same temperature (i.e., the Curie temperature T_c). The application of magnetic fields shifts the transition to the higher-temperature regime, causing a substantial reduction in resistivity near T_c and hence colossal MR. The origin of this effect is not well understood, although explanations have been discussed involving double exchange (DE) [3], electron–phonon coupling [4], orbital ordering effects [5], various polarons [6, 7] and a microscopic theory of electrical transport recently developed recently by Alexandrov and Bratkovsky [8]. In the present work, we report on the Monte Carlo simulations of resistance as a function of temperature and magnetic field based on the random-resistor-network model consisting of FM metallic particles and PM insulating particles. We show that using the reduced magnetization as the number density of FM metallic particles, the simulation can yield the main features of the colossal MR

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generally reported for the optimal manganese perovskites. Simulations are also performed for $(La_{0.8}Y_{0.2})_{2/3}Ca_{1/3}MnO_3$, showing an excellent agreement with experimental data.

It has been commonly believed that the perovskite-related manganites can accomplish a dynamic phase segregation [9]. Because of the phase segregation, it is likely for the optimal manganese perovskites that FM domains exist within the PM matrix for the temperature range $T > T_c$, while PM regions exist in the FM background for the temperature range $T < T_c$. Experimental evidence for the presence of short-range FM domains in the PM background can be found in experiments such as electron paramagnetic resonance [10] and small-angle neutron scattering measurements [6]. Experiments such as scanning tunnelling spectroscopy [12], magnetic force microscope [13] and electron microscopy [14] measurements, on the other hand, directly confirm the coexistence of FM domains and PM regions below T_c. According to the DE mechanism [3], the charge carriers with same spin orientations can move easily; therefore, the electrical conductivity is metallic in the FM state, whereas the electrical conductivity is insulating in the PM state because of disorder scattering from charge carriers with different spin orientations. It is therefore reasonable to assume that the sample is phase separated into a mixture of FM metallic domains and PM insulating regions.

On the basis of the above consideration, a phenomenological model for resistance as a function of temperature and magnetic field was recently proposed [11] in which the total resistance is represented as a sum of two contributions, from the PM insulating phase and the FM metallic phase. It is shown that this phenomenological model can quantitatively explain experimental observations for the optimal manganese perovskites; however, FM metallic and PM insulating regions are assumed to be electrically connected in series. Clearly, the connection in an actual system should be much more complicated than this assumed form. The actual situation should be that FM metallic and PM insulating regions randomly fill the space of the sample. In order to create such a distribution, the Monte Carlo method is used, which is described as follows.

We assume the sample to consist of dense grains of PM insulating particles and of FM metallic particles packed together so that the particle centres occupy the nodes (or sites) of a network lattice. Between each pair of particles i and j in the network lattice, current is conducted through a 'bond resistance' R_{ij}. The bond resistance R_{ij} is determined from the kinds of particle residing at sites i and j. Between each pair of particles of the same kind (FM metal or PM insulator), the bond resistance is the resistance of the corresponding particles themselves, i.e., $R_{ij} = R_{FM}$ (or R_{PM}). If the two sites are occupied by different kinds of particle, i.e., a FM metallic particle at site i and a PM insulating particle at site j, say, the bond resistance between sites i and j is determined by

$$\frac{1}{R_{ij}} = \frac{1}{R_{PM}} + \frac{1}{R_{FM}}. \tag{1}$$

The kinds of particle residing at sites i and j depend on the value of a computer-generated random number. If this number is smaller than the chosen number density (p) of FM metallic particles, the site is assigned a FM metallic particle. Otherwise the site is taken to be occupied by a PM insulating particle. Through this process, the random resistor network can then be constructed. Application of the Kirchhoff current law to each mesh then constitutes a set of equations that may be solved numerically by the Monte Carlo method.

Quite recently, Monte Carlo simulations of electrical conductivity in zero field were performed [15] for $(La_{1-x}Y_x)_{2/3}Ca_{1/3}MnO_3$ ($x = 0$, 0.1 and 0.2) using the random-resistor-network model mentioned above. The simulations show excellent agreement with experimental data over the whole temperature range covering high-temperature insulating and low-temperature metallic regimes. From these simulations, it has been shown that the transition

to a metallic state occurs as p (or f, the volume fraction of FM metallic phase) exceeds the percolation threshold (10–20%). This suggests that the transition to the metallic state is due to a percolation of FM metallic domains. In the present work, we shall show that upon the application of magnetic fields, the electrical conductivity can also be simulated through the random-resistor-network model mentioned above.

To perform the Monte Carlo simulation, we first need to know three quantities: R_{PM}, R_{FM} and p, which appear in the random-resistor-network model. As previously shown [11], both R_{PM} and R_{FM} can be approximated by $R_{PM} = R_0 e^{E_g/k_B T}$ and $R_{FM} = bT^2$. Since p represents the number density of FM metallic particles, it should be proportional to the reduced magnetization m. We therefore approximate p by m which can be determined from the mean-field theory. According to this theory, m can be expressed in terms of solutions of the mean-field self-consistency equation [16]

$$m(h,t) = B_J\left(\frac{3J}{J+1}\frac{m+h}{t}\right) \tag{2}$$

where B_J is the Brillouin function defined by

$$B_J(x) = \frac{2J+1}{2J}\operatorname{cotanh}\left(\frac{(2J+1)x}{2J}\right) - \frac{1}{2J}\operatorname{cotanh}\left(\frac{x}{2J}\right).$$

J is the angular momentum quantum number, t ($\equiv T/T_c$) is the normalized temperature, h ($\equiv H/H_e$) is the normalized magnetic field and H_e is the saturation exchange field. Assuming that the orbital angular momentum is quenched, the effective value of J is then calculated to be 1.83 for the optimal manganese perovskites of the form $Re_{2/3}B_{1/3}MnO_3$ with a mixture of Mn^{3+} ($S = 2$) and Mn^{3+} ($S = \frac{3}{2}$) ions. Taking $T_c = 90$ K, m (and hence p) as a function of T and h can then be obtained by solving equation (2). Shown in figure 1(a) is the thus-obtained p as a function of temperature for a range of normalized fields h from 0 to 0.16 in steps of 0.02.

Once the temperature dependence for the above three quantities is known, we can perform the Monte Carlo simulations of the magnetoresistance. The simulations are done on a two-dimensional (20×20) matrix using $T_c = 90$ K, $R_0 = 10^{-3}$ Ω, $E_g/k_B = 1000$ K and $b = 10^{-5}$ Ω K^{-2}. The simulated data are plotted in figures 1(b) and 1(c) in various given fields for the whole temperature range covering the high-T insulating behaviour and low-T metallic behaviour with a temperature step of 5 K. Clearly, the main features of the colossal MR generally reported for $Re_{2/3}B_{1/3}MnO_3$ can be found from this set of resistance curves indicated in figures 1(b) and 1(c). It is essential to note that the set of resistance curves is obtained only through increasing fields that cause increases in p, but with the other parameters (T_c, R_0, b and E_g) remaining unchanged. We therefore naturally suggest that the colossal MR originates mainly from the field-induced increase in the number density (volume fraction) of FM metallic particles.

To be convincing, we must show that we can yield quantitatively experimental data for the temperature dependence of the colossal MR through the Monte Carlo simulations. For this purpose, we have measured the temperature dependence of the resistance for fields of 0 and 5 T in $(La_{0.8}Y_{0.2})_{2/3}Ca_{1/3}MnO_3$. This sample is the same as that used in recent studies [15]. The experimental data are plotted in figure 2(a) (open circles). The simulation of the zero-field R versus T dependence has been presented elsewhere [15] using $R_{PM} = 4.34 \times 10^{-3} e^{1184.5/T}$ (Ω) and $R_{FM} = 1.0 \times 10^{-5} T^2$ (Ω). This is replotted in figure 2(a) as a function of temperature with the corresponding experimental data (open circles), where p is used as a fitting parameter which is plotted in figure 2(b) as a function of temperature. In figure 2(b), we also present a comparison between the p-values (solid circles) used in the simulation and the m (solid line) determined from equation (2) using $T_c = 87$ K and $h = 0$. It can be found that at temperatures slightly lower than T_c the p-values used in the simulation have the same values as those obtained

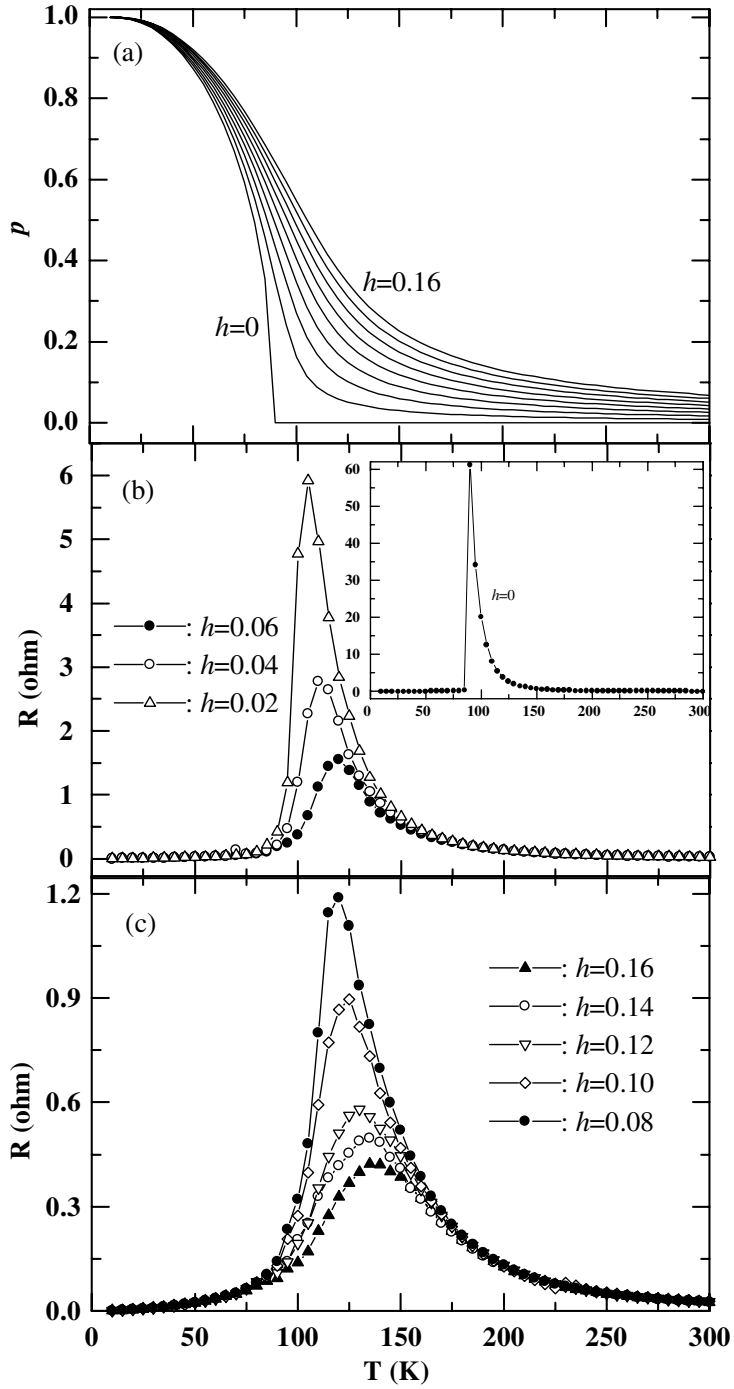

Figure 1. Temperature dependences of the number density of FM metallic particles (a) and of resistance ((b), (c)) for fields of $h = 0$–0.16 in steps of 0.02. p is calculated from the mean-field self-consistency equation with $J = 1.83$ and $T_c = 90$ K. Symbols in (b) and (c) represent resistance data at various representative fields which are obtained through the Monte Carlo method in temperature steps of 5 K using f-values indicated in (a); $R_{PM} = 1 \times 10^{-3} \mathrm{e}^{1000/T}$ (Ω) and $R_{FM} = 1.0 \times 10^{-5} T^2$ (Ω). The solid lines in (b) and (c) are drawn as guides to the eye.

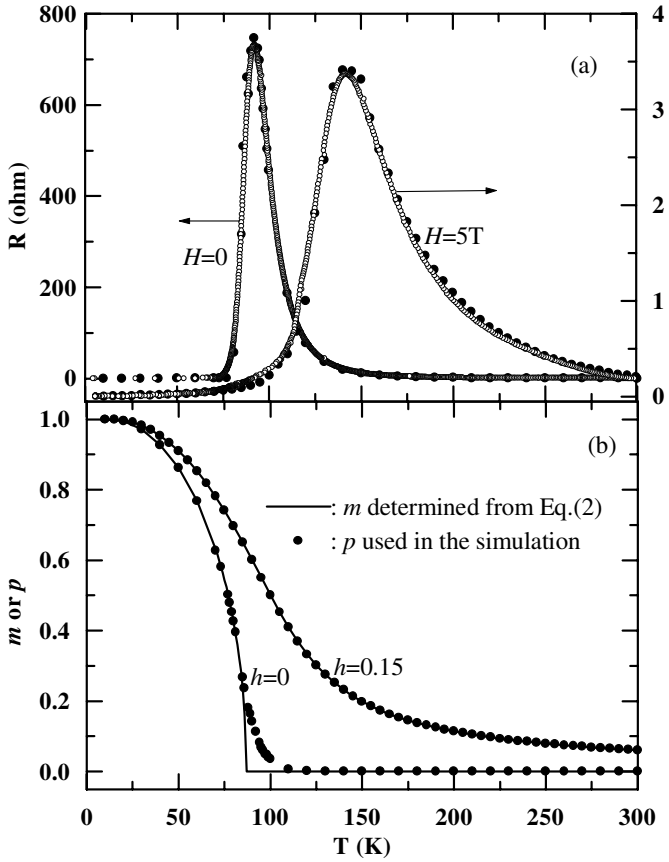

Figure 2. Temperature dependences of the resistance for fields of 0 and 5 T in the compound $(L_{0.8}Y_{0.2})_{2/3}Ca_{1/3}MnO_3$: (a) comparisons of the resistance between simulated (solid circles) and experimental (open circles) data and (b) comparisons between p used in the simulation (solid circles) and m determined from the mean-field theory (solid lines).

by the mean-field theory, but a larger difference between them exists at temperatures around T_c. This difference around T_c should be a consequence of dynamic phase segregation that creates short-range FM domains within the PM matrix. Detailed discussions for the case of zero field have been presented elsewhere [15]. In the present work, we will show that using these quantities (R_{PM}, R_{FM} and T_c) obtained from the zero-field data, the MR data can be quantitatively yielded through the Monte Carlo method.

For the case of applying the field, we directly use m as p in order to limit the randomness. Using $h = 0.15$, $J = 1.83$ and $T_c = 87$ K, p is calculated from equation (2) which is plotted in figure 2(b) as a function of temperature. The simulation is performed on a two-dimensional matrix of $N \times N$. We find that the simulated results clearly show a diverging behaviour for a smaller matrix with $N < 20$ but vary in a regular fashion for a larger matrix with $N \geqslant 20$. We therefore choose a 30×30 matrix for the present simulations. Using the p-values indicated in figure 2(b), we have performed the Monte Carlo simulation of resistance as a function of temperature for the field of 5 T. The simulated data (solid circles) with a temperature step of 5 K are superimposed on the corresponding experimental data (open circles) as indicated in figure 2(a). Indeed as seen in the figure, excellent agreement is obtained between the

simulated and experimental data for the whole temperature range studied. Here we emphasize again that in the present simulation, except for p, all other quantities are determined from zero-field resistance data such as $R_{PM} = 4.34 \times 10^{-3}\mathrm{e}^{1184.5/T}\ \Omega$, $R_{FM} = 1.0 \times 10^{-5}T^2\ \Omega$ and $T_c \sim 87$ K. Making a comparison between p-values for fields of 0 and 5 T, it is clear that the colossal MR originates mainly from the field-induced substantial increase in the volume fraction of FM metallic phase.

In summary, we have shown that the colossal MR can be quantitatively explained by considering that FM metallic and PM insulating regions randomly fill the space of the sample. The Monte Carlo simulation of magnetoresistance yields the main features of the colossal MR generally observed in doped manganese perovskites and shows excellent agreement with experimental observations on $(La_{0.8}Y_{0.2})_{2/3}Ca_{1/3}MnO_3$. The essential conclusion is that the colossal MR originates mainly from the increase in the volume fraction of the FM metallic phase caused by the application of the fields. Further understanding is needed for the mechanism of formation of the FM metallic phase within the PM insulating matrix and the physical basis of the present approach, which will be given elsewhere.

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