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Heating and non-ohmic transport in phase-separated manganites

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Abstract. We investigate the features of non-ohmic transport in phase-separated manganites by Monte Carlo simulations in a random network with clusters of ferromagnetic metal and antiferromagnetic insulator. It is found that, by taking into account the heating process and the temperature dependence of resistivity, the current-voltage characteristics are highly non-ohmic and exhibit hysteresis in sweeping the voltage. We calculate the temperature dependence of this behavior, and investigate the changes of the percolative paths at different currents. The breakdown of most percolative paths by the heating effect of the current results in an interrupt transition from the metallic behavior to the insulator behavior of the system. The obtained results are in good agreement with related experiments.

PACS. 75.40.Mg Numerical simulation studies – 75.50.-y Studies of specific magnetic materials – 64.60.Ak Renormalization-group, fractal, and percolation studies of phase transitions – 64.75.+g Solubility, segregation, and mixing; phase separation

1 Introduction

Recently, the manganites, as materials of colossal magnetoresistance effect (CMR), have become a focus of investigations in condensed matter physics for their curious properties as well as possible applications in technology. There are already several theories relying on mechanisms such as Anderson-localization induced metal-insulator transition [1] and the gas of correlated polarons, attempting to explain the complicated phase diagrams of these compounds. It seems that the phase separation (PS) scenario [2,3] may provide results compatible with a large number of experimental data, and the existence of PS has been widely accepted due to the intrinsic quenched disorder in these compounds.

For manganites, one of the important issues is to study their transport properties which crucially depend on the structures of PS. According to results of experiments, there are two classes of PS structures, the microscopic (nanometer scale) PS and the mesoscopic (micrometer scale) PS [4]. For materials with the first class of the PS, it is difficult to calculate their properties because of its microscopical inhomogeneity in the space. The coexisting clusters of micrometer sizes observed in experiments suggests that the PS in some materials is of the second class and the phenomenological or classical approaches can be adopted in the study of properties. In this aspect series of studies have been carried out to calculate the dc resistivity ρ_{dc} in the mix-phase regime using a random resistor network model (RRN) [5,6]. This model was introduced initially in the study of metal-semiconductor transitions in CMR materials. It consists of a square or cubic lattice whose links represent metal or insulator clusters with different resisters distributed according to the ratio of metal to insulator clusters in the PS manganites. For a specific cluster, the resistivity or conductivity is usually a function of temperature T. When the temperature is fixed for all the clusters, the resistance of the whole system is a constant and an ohmic $V - I$ relation is expected in the RRN models. Recently, however, Tokunaga et al. reported that an abrupt jump and hysteresis behavior in $V - I$ characteristics in the mesoscopically phase-separated material $[(La_{0.3}Pr_{0.7})_{0.7}Ca_{0.3}MnO_3]$ may occur when the total current reaches a threshold value I_{th} [7]. The ohmic relation is observed only when the current is smaller than I_{th} and the temperature is below the ferromagnetic (FM)-antiferromagnetic (AFM) transition. They guess that the abrupt change of voltage by applying large amounts of current can be ascribed to the collapse of metallic channels caused by the temperature rising due to the heating process. Besides these, the experimental results also show an hysteresis phenomenon in both $\rho - T$ and $V - I$ curves, which are considered as an indication of the changes of PS patterns in sweeping the temperature or current.

To investigate these interesting phenomena, we suggest a modified RRN model from which the temperature

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dependence of the resistivity and the heating process can be taken into account in the simulations. Since the spirit of the RRN model is to simulate the inhomogeneously distributed clusters of different phases inside the real material, the intrinsic properties of the compound, such as the temperature dependence of resistivity, can be assigned to individual clusters. The properties of the whole system can be obtained from the average values in the simulation of all the clusters. In this way we reproduce the non-ohmic voltage-current curves in our simulations. By considering the general rules in the first-order phase transition [8], we also obtain the hysteresis in both $\rho - T$ and $V - I$ curves. The results are in good agreement with the experiments.

2 Model and formulism

We use a three-dimensional cubic lattice to construct the RRN model for the bulk materials. Just like other non-correlated RRN models, in the 3D cubic lattice the FM metallic clusters and the AFM insulating clusters occupy the nodes of the lattice, and the bond resistance R_{ij} connects nearest-neighbor (NN) nodes i and j. The bond resistance R_{ij} is determined by the type of clusters at nodes i and j. If the NN nodes are both FM metal or AFM insulator, the bond resistance R_{ij} connecting them is R_{FM} or R_{AFM} in accordance with their type. If the NN nodes are not of the same type, the resistance R_{ij} is $R_{FM}R_{AFM}/(R_{FM} + R_{AFM})$. With the number density P of FM metallic clusters we can create realizations of the RRN using a random-number generator. The number density P is proportional to the reduced magnetization m. From the molecular field theory, m, as a function of the normalized temperature t ($\equiv T/T_c$ with T_c being the Curie temperature) and magnetic field h ($\equiv H/H_e$ with H_e being the saturation exchange field), can be approximately determined by the self-consistent equation [6,9],

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

where $B_J(x)$ is the Brillouin function

$$B_J(x) = \frac{2J+1}{2J}\mathrm{cotanh}\left(\frac{x(2J+1)}{2J}\right) - \frac{1}{2J}\mathrm{cotanh}\left(\frac{x}{2J}\right), \tag{2}$$

with J being the angular momentum quantum number. The normalized magnetic field h equals to zero because no external magnetic field is considered here. For a material such as $(La_{0.3}Pr_{0.7})_{0.7}Ca_{0.3}MnO_3$, the temperature dependence of the resistivity of FM-metal phase and AFM-insulator phase can be fitted by $\rho_{FM} = c_1T^2$, with $c_1 \simeq 1.28 \times 10^{-5}\,\Omega\mathrm{cm\ K}^{-2}$, and $\rho_{AFM} = c_2e^{c_3/T}$, with $c_2 \simeq 4.60 \times 10^{-3}\,\Omega\mathrm{cm\ K}^{-2}$ and $c_3 = 1.55 \times 10^3$ [9–11]. With this RRN model we can study the transport properties by solving the Kirchoff equation based on the relaxation technique. According to the results of experiments, we choose the transition temperature from the FM-metal $T_c \simeq 140$ K in the heating process and $T_c \simeq 130$ K for the cooling process.

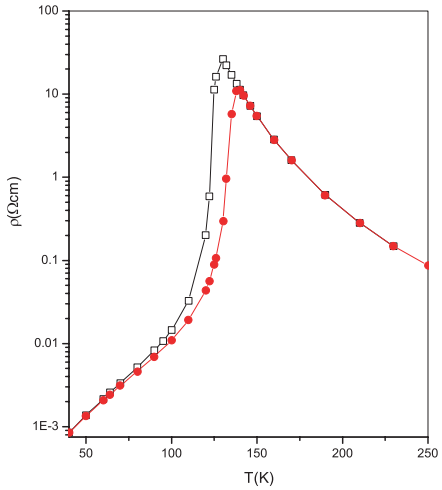

Fig. 1. Temperature dependence of resistivity for $25 \times 25 \times 25$ cubic lattice in heating (closed circles with $T_c \sim 140$ K) and cooling (open circles with $T_c \sim 130$ K) processes.

3 Simulation results

With the formulism mentioned in the last section we carry out the Monte Carlo simulations on a $25 \times 25 \times 25$ cubic lattice from which the average resistivity and the $V - I$ characteristics can be obtained. In Figure 1 we plot the temperature dependence of the average resistivity in both the heating and cooling process. From Figure 1 the first-order phase transition between the FM-metal phase and the AFM-insulator phase in both heating and cooling processes can be seen. At temperatures below the T_c, the resistivity increases with increasing the temperature, corresponding to the metallic behavior. By further increasing the temperature it rapidly reaches the maximum value at T_c, and then decreases in region $T > T_c$, indicating the first-order transition from the metal to the insulator. The transition temperature is different for the heating and cooling processes from the assumption of different Curie temperatures for the magnetic properties. Apart from T_c the curves for these two processes almost merge together, and the difference appears only near T_c. The rapid jumps of resistivity near T_c is from the breaking of the percolative paths due to the reduction of the metal clusters. This behavior can be understood from the temperature dependence of the number density of the FM-metal clusters shown in Figure 2. It can be seen that by increasing the temperature from below T_c to above T_c the number density of metal clusters is rapidly decreased to a vanishing value. Apart from T_c, there is almost no difference in the number density between the heating and the cooling processes.

Although the metal and insulator clusters coexist in the model, at a low (high) temperature, the metal (insulator) regions take up the majority percentage of the lattice. As a result, the conduction is mainly through percolative metallic (insulator) channels and the lattice shows metallic (insulator) behavior. Once the temperature is above T_c, all the metallic paths are nearly broken, and the net

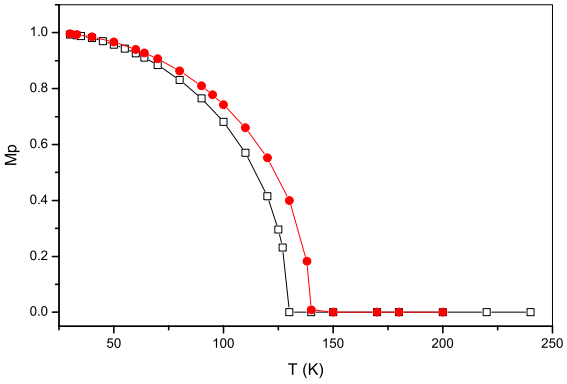

Fig. 2. Temperature dependence of number density P of FM metallic clusters for $25\times25\times25$ cubic lattice in heating (closed symbols with $T_c \sim 140$ K) and cooling (open symbols with $T_c \sim 130$ K) processes. The bath temperature is given in the legend.

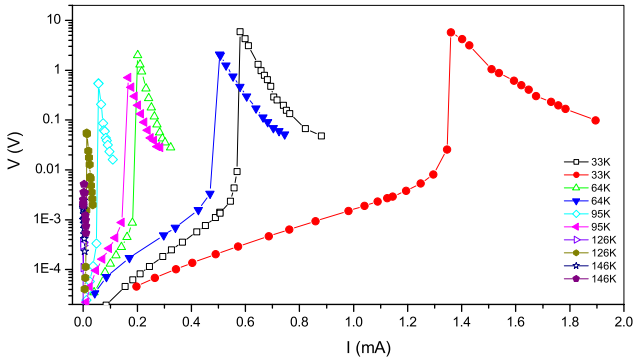

Fig. 3. $V-I$ curves at various temperatures for $25\times25\times25$ cubic lattice in current-increasing (closed symbols) and current-decreasing (open symbols) processes.

resistivity of the material behaves like a insulator. This is the first-order phase transition in a percolative network. The curves from the simulation of the present RRN model are in consistence with the results of the experiment [7].

Usually from the above model we can get a constant resistivity at a given temperature and the $V-I$ curves should be ohmic. However, the experiment [7] shows that this is not always correct. In fact, the $V-I$ curves in the experiment are non-ohmic. The ohmic behavior exists only when the current is well below some threshold value. If the current is near the threshold value, an increase of the current causes a steep jump of the voltage, corresponding to an increase of the resistivity by more than 3 orders of magnitude.

To explain this phenomenon, we consider the heating processes in the material due to the applied dc current. If a current I is flowing through the system and the voltage is V, a heat quantity $Q = IV$ per unit time will be created in the system. At the same time the reduction of heat quantity in a unit time by the thermal transmission should be $Q = k(T - T_0)$, where T and T_0 are the temperatures of the system and the bath, respectively, and k is the thermal conductance between them. From the steady condition one can determine T from the current and the voltage. As the local resistivity and the total percentage of clusters is dependent on temperature T and their kind as well, we should carry out a self-consistent calculation in the Monte Carlo simulation to determine the total current. For this purpose the thermal conductance k is necessary. This is usually not available. We will set the thermal conductance as a parameter which can be fitted from the experimental data. Considering that in the process of heating by the current the surrounding materials have lower relative temperature than that in the cooling process, the effective thermal conductance between the system and the bath should be larger in the heating process than that in the cooling process. From the experimental data we choose $k_1 \sim 1.44\times10^{-6}$ watt/K for the heating process and $k_2 \sim 2.95\times10^{-7}$ watt/K for the cooling process. When we increase the current at a given bath temperature, the system will heated and the temperature T will rise. On the contrary, when we decrease the current, the temperature of the system will be decreased. Consequently the resistivity of the system becomes current dependent and the $V-I$ curves exhibit non-ohmic behavior.

In Figure 3 we present the simulation result of the $V-I$ curves at different bath temperatures in both current-increasing and current-decreasing processes. When the bath temperature is lower than T_c, in both processes there is an obvious threshold current I_{th}, below which the $V-I$ curves are nearly ohmic. At I_{th} a steep increase of the resistivity by about 3 orders of magnitude occurs. Above I_{th} the $V-I$ curves are highly non-ohmic. I_{th} is smaller in the current-increasing process than in the current-decreasing process. All these characteristics are compatible with the experiment. When the bath temperature is high enough, the ohmic region of the current almost disappears. The different behavior in current-increasing and current-decreasing processes originates from the different effective thermal conductance and different Curie temperature. This results in the hysteresis in the sweeping of the current observed in the experiment [7]. The hysteresis behavior is possibly associated with the first-order transition in which the hysteresis in cycling through the transition and the accompanying effects of superheating and supercooling often happen [12]. In $(La_{0.3}Pr_{0.7})_{0.7}Ca_{0.3}MnO_3$, the fact that the transition from the FM-metal phase to the AFM-insulator phase occurs at temperature higher than that of the reverse transition, is just a demonstration of this general feature of the first-order transition.

At low temperatures most of the clusters are metallic. Therefore, the applying of a small current can not produce enough heat to break the percolative paths. As a result, the ohmic relation remains. A large current will produce enough heat to increase the system temperature up to T_c, and almost all the metallic paths are rapidly broken, resulting in non-ohmic behavior. I_{th} decreases by increasing the bath temperature. In Figure 4 we show the spatial distribution of the local current density, from which the breaking of the metallic paths in increasing the current can be seen.

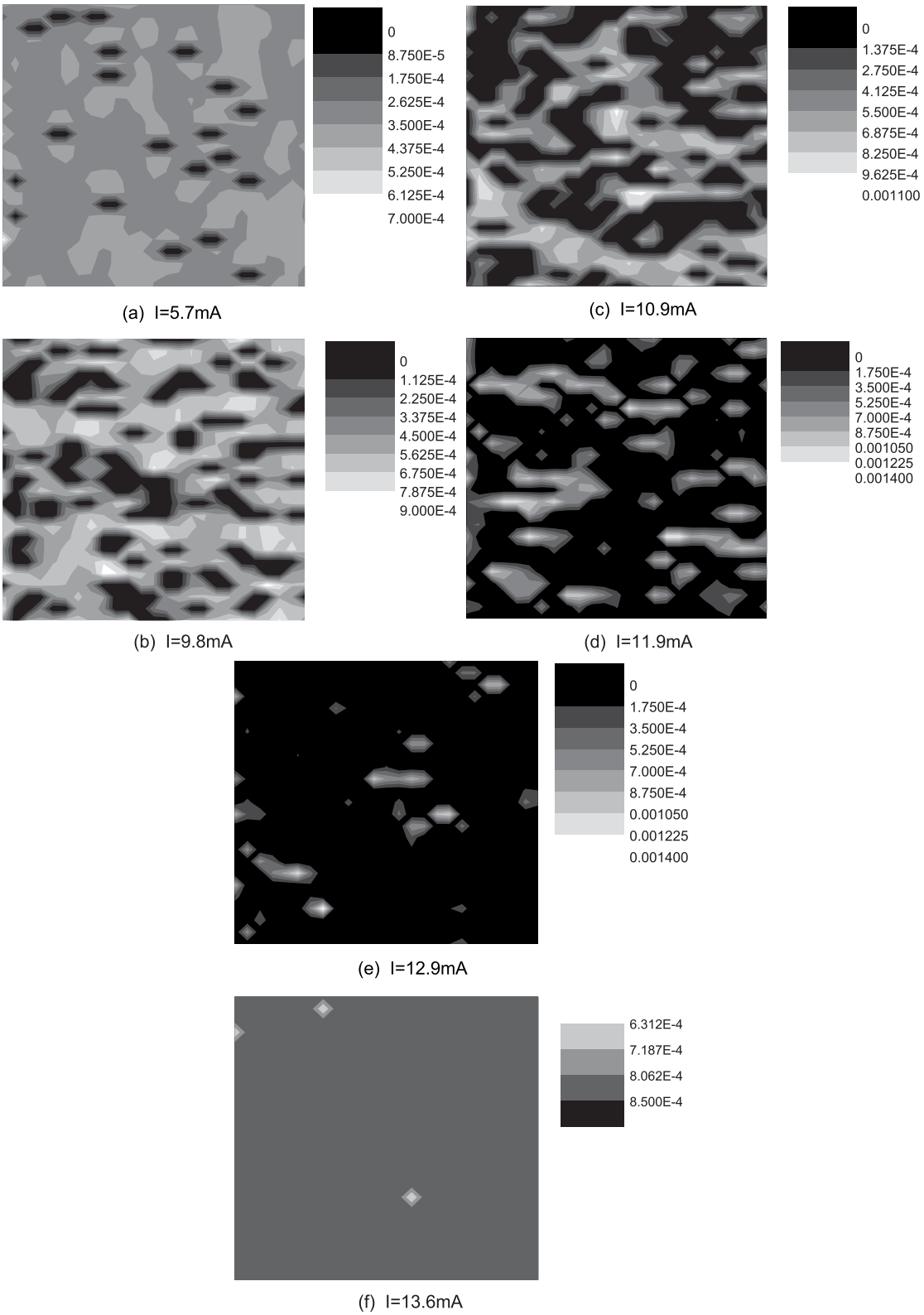

Fig. 4. Distribution of local current density in a middle layer of a $25 \times 25 \times 25$ in the process of current increasing. The units of in-plane current density is Volt/(Ωcm). The bath temperature is $T_0 = 33$ K. The total current is given at the bottom. Other parameters are the same as those in Figure 3.

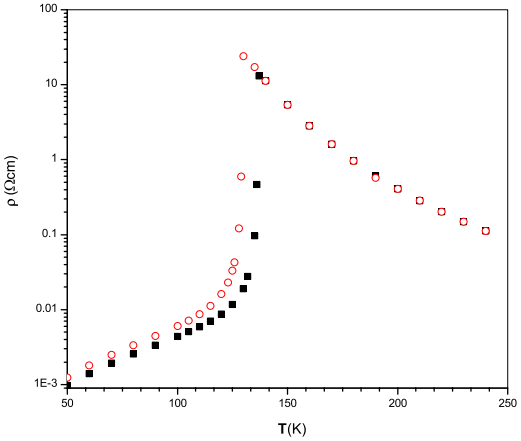

Fig. 5. $\rho - T$ curves at various temperatures for the correlated RRN on a $25 \times 25 \times 25$ cubic lattice in heating process (closed symbols) and cooling process (open symbols) considering the different transition temperature.

On the other hand, it is wildly believed that micrometer scale PS is driven by disorder near the first-order metal-insulator transition. It has been suggested that the correlated occupation of metallic clusters could be used to explain the hysteresis effect [12]. From this point of view we construct a correlated RRN model in such a way that the probability of adding new metallic (or insulating) cluster at a certain site is larger when there are already metal-occupied sites adjacent to it. We find that even in such a correlated RRN model the hysteresis can occur only by introducing different transition temperatures for heating and cooling processes. This is illustrated by Figure 5 showing the simulation result on the correlated model. It is essentially the same as that for the uncorrelated model shown in Figure 1. This means the view based on the correlated conglobation in such PS materials may not be suitable to explain the hysteresis phenomenon, although it seems to be a reasonable one to explain the "overshot" hysteresis in [12].

4 Conclusions

In this paper, considering the general character in first-order phase transition, we use different T_c to simulate the $\rho(T)$ curves in heating and cooling processes. We also study the non-ohmic $V - I$ curves with the generalized RRN model including the heating effect of the current. From the heating effect and the $\rho - T$ characteristics, we find that the applying of the current has the same role as the increasing of the temperature in inducing the collapse of the percolative paths in the phase-separation state of the manganite materials. This collaspe is directly reflected in the abrupt jumps in $V - I$ curves and the non-Ohmic $V - I$ relation. The simulation results are qualitatively consistent with the experiment. The mechanism inducing the hysteresis in this material needs further investigation, for it seems that the view based on the correlated conglobation in this PS material could not provide a good result in the simulation on the correlated RRN model.

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