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The effects of current-path patterns on magnetotransport in spatially-confined structures by Monte Carlo simulation*

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Simulations are performed on clusters of finite size to study the effects of size and current-path structure on magnetotransport in spatially-confined samples. Magnetotransport networks are established and calculated based on fractal structures including Koch curves and percolation backbones extracted from regular lattices. The structure pattern of clusters is shown to play an important role in the magnetotransport behaviours by affecting the magnetoresistance fluctuations due to spin disorder in the systems of small size, which suggests the possibility of controlling the magnetotransport by the design of current-path configurations.

Keywords: magnetoresistance, percolation, magnetotransport network

PACC: 7570, 7540, 7155

1. Introduction

Recent studies of spatially-confined structures of magnetoresistance (MR) materials have revealed the importance of the underlying current paths on macroscopic MR behaviours.[1−5] Various MR materials, ranging from phase-separated CMR manganites to nanoconstricted ferromagetic granular systems, have been reported to exhibit interesting magnetotransport properties as well as higher sensitivity when the sample size is reduced to a mesoscopic scale. The interesting magnetotransport properties emerging with decreasing size of these sample are interpreted as a size effect of magnetotransport within a percolation cluster: the currents tend to be driven into a spanning cluster by disorder and shrinking size diminishes the possibility of multichannels within the clusters. In the limiting case, a single quasi-one-dimensional current path,[2,4] the most advantageous structure for MR, is formed. This 'smaller-size-fewer-channels' scenario, though simple and qualitative, has served as a good basis for understanding the magnetotransport properties observed in these spatially-confined structures, such as the field-dependent multisteps of negative differential resistance.[1,5]

However, a percolation cluster is certainly not just 'a few channels'. Studies for decades have been devoted to revealing the complicated internal structure of these clusters, especially the incipient one occurring at the percolation threshold.[6−9] Finite-size, according to statistics of numerous samples, not only means a finite number of conducting paths but also affects the geometric patterns of these paths.[7] This combined effect of size and structure is well-known for its crucial role in many physical properties, such as electrical transport or elasticity, of the clusters. But little is known so far about how it influences the magnetotransport behaviours of the clusters, to what extent and in which way.

This question is not only important to understand the MR behaviours of mesoscopic samples. With the rapid development of nanofabrication techniques, it can be expected that an insight into the relation between finite cluster structures and magnetotransport properties may open a gateway to new MR functionalities by geometric designs of current-path patterns in these materials. Motivated by these considerations we performed Monte Carlo simulations on finite clusters with different structures to get this important insight. The results from two types of structure patterns are presented in this paper: one is the percolation backbones in square or cubic lattices and the other is the Koch curves, one of the famous deterministic fractals. Both the structures possess the important features of spanning clusters formed in real materials, such as fractal dimensions or the existence of 'key'

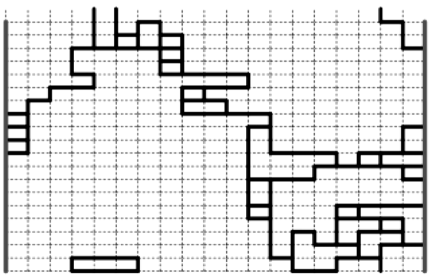
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bonds in magnetotransport,[2] and can be described by the well-known 'links-nodes-bulbs' model.[6] The results show clearly the structure-dependence of the MR fluctuations due to magnetic disorder in systems of small size, which offers a new route to improve the MR behaviours by tailoring the current-path patterns in spatially-confined structures.

2. The network models

We begin by creating incipient percolation clusters in two-dimensional(2D) square lattices and three-dimensional(3D) simple cubic lattices. The bonds are occupied at probability $p = 0.5$, the exact percolation threshold for the 2D cases, and $p = 0.2488$, the numerical estimation for the 3D cases.[6] The conventional bus-bar geometry is adopted, where the percolation clusters are operationally defined in a box of edge L as the largest cluster connecting a pair of bars attached to the opposite sides of the box. In the simulations we first identify the percolation clusters using the Hoshen–Kopelman algorithm[10] and then extract the backbones by the direct electrifying algorithm.[11] The size effects are studied with L varying from 10 to 200. Figure 1(a) illustrates a typical backbone structure obtained in a 2D square lattice for $L = 20$.



(a)



(b)

Fig.1. (a) The backbone structure extracted from a 20×20 square lattice in the simulations. (b) The third generation of a Koch curve with possible current paths as defined in the main text.

To establish a magnetotransport network based on the backbones as obtained above we choose the conventional expression of spin-polarized tunnelling conductance[12] to describe the bond joining adjacent sites i and j

$$G_{ij} \propto (1 + P^2 \cos\Theta_{ij}) \exp(-2\kappa s), \qquad (1)$$

where κ and s describe the height and width of tunnelling barriers respectively while Θ_{ij} is the relative angle between the orientations of the magnetic moments on adjoint sites. Each site of the cluster is denoted by a local magnetic moment with uniformly-distributed orientation in the absence of magnetic fields. Note that this spin-polarized tunnelling mechanism has been successfully applied to the typical TMR behaviours for ferromagnetic granular metals[12] and polycrystalline half-metals.[13,14] Since in this work we try to focus on the effects of underlying current configurations on total magnetotransport instead of details in microscopic transport processes, we choose this magentotransport mechanism due to its simplicity and sufficiency to reveal the basic characteristics of the response of individual bonds to magnetic fields. Spin polarization of the charge carriers P reflects the sensitivity of individual bonds to magnetic field and, when a saturation field H_s is applied, all the magnetic moments align in parallel so that $\cos\Theta_{ij} = 1$. To obtain the cluster conductance at different fields a unity potential difference is set between the bars. Then we store the coefficient matrix of the Kirchhoff equations with the row-indexed compact storage strategy and solve the matrix with the biconjugate gradient method. The MR ratio of the total cluster is calculated using

$$\mathrm{MR} = \frac{G(H) - G(0)}{G(H)}, \qquad (2)$$

where $G(H)$ and $G(0)$ are the cluster conductances with and without the applied field respectively.

3. Numerical simulations and results

The MR ratios of the backbones in 2D systems with $L = 200$ (2DBB) and in 3D systems with $L = 40$ (3DBB) are displayed in Fig.2 together with the results for regular lattices. For full spin polarization $P = 100\%$, namely the ideal half-metallic materials, the average MR ratios realized in the backbone structures reach 0.86, much higher than 0.57 in 3D regular lattices and 0.62 in 2D regular lattices. This result confirms the previous prediction that a percolation

cluster structure can induce dramatic MR enhancement, especially for half metals. A similar behaviour is also observed for other systems with high spin polarization $P > 0.5$, as shown in the inset of Fig.2.

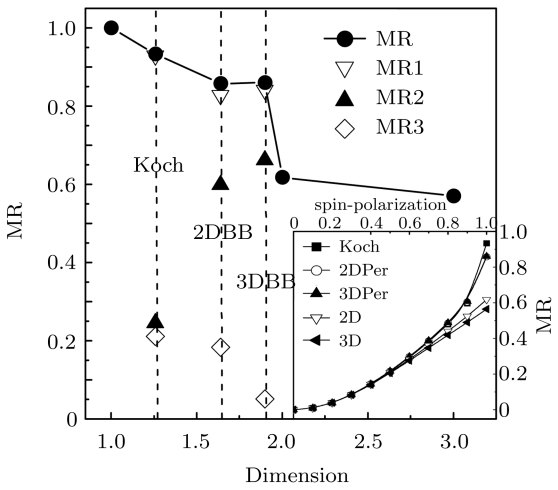


Fig.2. The MR ratios vs the dimensions of different structures for $P = 1$, where the 'MR' data refer to the results from the total cluster and MR1, MR2, MR3 are defined in the main text. The inset shows the dependence of the MR values on spin polarization.

Next we investigate the influence of the internal structure of a percolation cluster on the magnetotransport behaviours. Generally, the backbone of an incipient percolation cluster can be viewed as a topologically linear 'pearl-necklace',[7] where the 'pearls' are the blobs, i.e. the multiply connected bonds, of different shapes and sizes, and the connecting strings of different length are composed of the links, i.e. the singly-connected bonds (SCB). This is the well-known 'links-nodes-bulbs' model.[6] To exhibit the contributions of the multi-connected sites in the bulbs to magnetotransport, the following procedure was performed. We first labelled each site according to the number z of its connected neighbours. Then we (i) killed the local spins on the sites with $z > 3$; (ii) killed the local spins on the sites with $z = 3$; (iii) killed all the local spins and then revived those on the site $z > 3$. The corresponding MR ratios, MR1, MR2 and MR3, are displayed in Fig.2. For both 2DBB and 3DBB, MR1 is very close to the total cluster MR but MR2 drops obviously, showing that the backbone magnetotransport is much more sensitive to the magnetic state of the 3-connected sites. After step (iii), all the link magnetotransports are suppressed and MR3 is just the contribution of the bulbs due to the revival of the local spin on multi-connected sites. The difference in MR3 between 2DBB and 3DBB is obvious, where 18.4% of the total MR is recovered for the 2D cases while only 5.1% is for 3D. This result is reasonable when considering the structure characteristics for different dimensions. Previous simulations have shown that the frequency of the occurrence of a long string of links is higher in the backbones of 3D systems than in those of 2D systems.[7] In this sense the backbone structures look more like a 'quasi-one-dimensional' path in higher dimensions, where longer strings connect diluted bulbs, and the sensitivity of the total magnetotransport to the multi-connected sites is obviously lowered.

To further exhibit the structure dependence of magnetotransport within a cluster, we established another magnetotransport cluster based on a deterministic fractal, the Koch curves, where the geometric structure is generated at each generation by replacing the line segment in the pre-generation with four line segments of equal length and iterating this process endlessly. The magnetotransport model is also based on the spin-dependent tunnelling between magnetic moments and transport is only allowed between nearest neighbours. Figure 1(b) shows the third generation of the Koch curve structure with all the possible transport paths displayed. Similar to the backbone structures, the Koch curves can also be viewed as a 'links-nodes-bulbs' model, but now the string of links is very short and the bulbs possess much more regular shapes and sizes, all with triangles as their building blocks. The same calculation procedures were performed on the Koch-curve-based magnetotransport networks and the results for the seventh generation are displayed in Fig.2. The behaviours are similar to those of the backbones except for a dramatic drop of MR2. This result is obviously due to the structure characteristics of the Koch curves where the link strings are so short that almost all of the link conductance is affected by the 3-connected sites located on the borders.

Now we can deduce that, though sometimes the underlying geometrical structure seems to contribute little when only the average MR of a total cluster is examined (for example, the total MR ratios of 2DBB and 3DBB shown in Fig.2 are very close despite the difference of structures), the contributions of the local magnetic moments on the multi-connected sites, especially of the 3-connected ones, are still obviously structure-dependent. Consequently, a structure-dependent sensitivity can be expected of intracluster magnetotransport to the arrangement of the on-site spins in the magnetic-disordered state. A direct proof of this property is the structure-dependent MR fluc-

tuations among samples with different magnetic configurations at $H = 0$ as observed in our simulations (Fig.3). Note that this is particularly important for small systems where the fluctuation is so obvious that broad MR distributions instead of average values are used to characterize the MR behaviours.

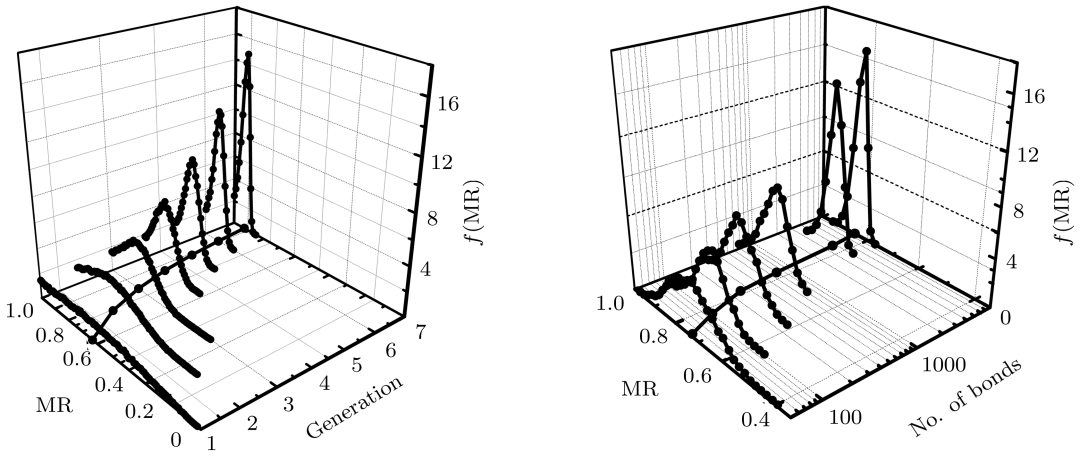


Fig.3. The probability density function of MR, f(MR), due to spin disorder of (a) the first–seventh generations of Koch curves. (b)the 2D backbones extracted from the square lattices with $L = 10, 20, 40, 80, 140$ and 200. The average MR values of each distribution are displayed by the squares on the bottom.

Figure 3(a) shows the probability distributions of MR due to magnetic disorder for Koch curves from the first to the seventh generation and Fig.3(b) for the typical backbone structures extracted from square lattices of L from 10 to 200. Here 'typical' means those backbones having the peak of the probability density near the average MR over all geometrical backbone configurations. The effect of cluster structure on the shape of the MR distributions is easily seen. For example, the high end of the distributions, i.e. the probability of higher MR ratios, is obviously raised in the cases of Koch curves when compared with the results from the backbones.

Figure 4 illustrates how the introduction of bulbs according to the Koch rules reshapes the probability density curves of the 1D string structures. The evolutions of the MR behaviours of both the string part and the total cluster are displayed from the first to the seventh generation. Size effects are obvious here. For generation 4–7 (right column), the string MR lies within the range of 0.6–1.0 and the probability density peaks are broadened and pushed to the left slightly after the bulbs are added to the cluster. However, for the lower generations (left column) where the number of bonds is less than 50, the long tails of the string-MR distributions extending into the lower-MR regime are suppressed by the bulbs, resulting in a narrowed peak in the total-cluster results.

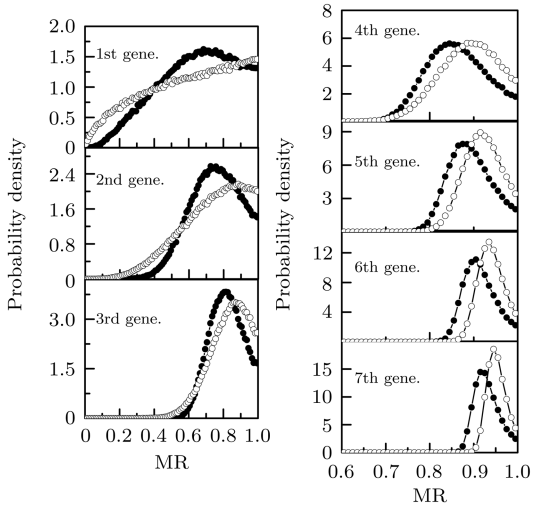


Fig.4. The evolution of the MR distributions of the total cluster (squares) and the corresponding string part (circles) from the first to the seventh generations of the Koch curves.

As statistical fractals, the backbones possess additional geometric fluctuation besides magnetic disorder. The obvious deviation of the MR distributions in Fig.3(b) from those of string MR (e.g., the vanish-

ing possibility of 100% MR of the backbones) shows the possibility of the existence of percolation clusters where the SCBs are not dominant even for small systems, though on average the portion of SCBs increases as size decreases.[6] Due to the large geometric fluctuation numerous samples are needed to obtain a complete description of the MR behaviours of the backbones of small sizes, which will be included in our future work.

4. Conclusions

In conclusion, the present work has provided an insight into the important role of size and structure patterns on magnetotransport of spatially-confined structures. Generally, a smaller size always tends to diminish the average MR while it enlarges the fluctuations among the samples with different magnetic configurations. However, better MR behaviours can be obtained by designing the structure patterns of clusters 'properly'. We give Koch-curve based clusters as an example to get MR distributions characterized by a raised high-MR end when compared with the naturally generated backbones in percolation systems. This feature is actually inherited from the MR behaviours of the SCBs as shown in Fig.4, and the introduction of the Koch bulbs always tends to keep the fluctuation of the cluster MR from extending into the low MR regions when the size is too small. Note that in this initial study we have only considered a randomly-oriented spin-disorder state and a magnetically-saturated state in calculation. If the interaction between local spins is taken into account to determine the local-spin configurations with or without field, more fractal-related effects on the MR behaviours of small clusters may be observed due to the special magnetic properties of fractal networks.[15−17] Hence we hope that this work will stimulate more interest in the effects of different artificial fractal structures of finite size on the intracluster magnetotransport, so that the geometric-pattern design can become a new effective approach to control the MR behaviours of mesoscopic samples for applications.

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