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LETTER TO THE EDITOR

Non-monotonic conductivity in a conductor-insulator fluid mixture

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Abstract. Charge transport in a stirred percolating system of a conductor-insulator mixture (a model for the microemulsion) is studied by computer simulation in two dimensions. The flow of charge from source to sink via nearest-neighbour charge exchange on the transient network of the conducting particles is considered. For the particle jump accompanied by a local charge transfer, the conductivity depends non-monotonically on the concentration p of the conducting particles and exhibits a maximum near the percolation threshold. The maximum vanishes and the conductivity rises with concentration p with a non-universal power on increasing the frequency of charge exchange.

Recently there has been increasing interest in studying transport phenomena, particularly diffusion and conductivity, in immiscible fluids modelled by stirred percolation [1-8]. In a conductor-insulator binary mixture [9], one of the most addressed questions by computer simulation [3-5] as well as by analytic methods [4, 5, 7, 8] is: how does the conductivity depend upon the concentration of the conducting constituents? To address this issue let us consider such a binary mixture of conducting particles A and insulating particles B , of concentrations p and $1-p$ respectively, distributed randomly on a discrete lattice where no site at any time can be occupied by more than one particle. Sites occupied by A particles provide paths for conduction and are called occupied sites while those sites occupied by B particles are called vacant as they block the conduction. Conducting particles are in constant stochastic motion and so are their vacancies, the particles at the B sites in a correlated fashion (see the model described below). A particles, starting at one end, have a finite probability of reaching the other end as long as p is non-zero. In most of the previous studies it was found that the conductivity increases monotonically on increasing the concentration p as the probability of forming the larger transient conducting network increases with the exception of interacting diffusion in static percolation [10, 11]. Above the percolation threshold p_c , there is at any fixed moment an infinite transient path which extends from one end of the system to the other. The conductivity increases as a function of p as the number of transient paths increases. Thus in the previous studies [3, 5, 7], the monotonic increase of the conductivity with concentration p was accounted for by the number of conducting paths where the details of the charge transport mechanism was not emphasised. Here, we present a computer simulation model for the charge transport in addition to particle transport in such a stirred system; this model shows

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a non-monotonic dependence of the conductivity on the concentration of the conducting particles.

We consider a two-dimensional lattice of N sites with $N = L_x L_y$, where L_x and L_y are the length and width of the system. At a concentration p , we randomly distribute $N_a (= pN)$ numbers of A particles with one particle per site. One end, say the left end, of the sample is connected with a source of charges while the opposite end (the right side) is grounded with the sink of zero charge. Each set of particles is assigned a charge density; particles in contact with the left end are assigned unit charge density, those in contact with the sink are assigned zero charge density and the rest of the mobile particles in the bulk are assigned a charge density of half initially. To maintain the charge neutrality there are always negative charges (equal in number) in the system but we are not considering them here for simplicity. All these N_a particles attempt stochastic motion with one attempt at random hopping by each particle per unit time step which is implemented as follows: we choose one of the N_a particles, say at site i and one of its neighbouring sites j randomly. If site j is vacant then the particle at site i is moved to site j and therefore the vacancy is automatically moved from site j to site i . On the other hand, if site j is occupied, then the particle stays at site i but the time step is increased in either case. A jump is accompanied by a charge transfer. Suppose the particle of charge density ρ_0 has hopped from site i to site j which has n nearest neighbours of charge densities $\rho_1, \rho_2, \dots, \rho_n$, then the charge density of all these $(n+1)$ sites (i.e. the site at j along with its neighbours) becomes $\rho = (\rho_0 + \rho_1 + \rho_2 + \dots + \rho_n) / (n+1)$. (Here, on the 2D lattice n varies between zero and three.) Of these $(n+1)$ particles, those in contact with the source (i.e. the leftmost column of the lattice) have their densities set to unity and the charge transfer $(1 - \rho)$ for each site is added to the total charge released from the source; those particles in touch with the sink have their densities set to zero and the charge transfer ρ for each site is added to the total charge absorbed by the sink. The whole process of (i) randomly choosing a particle, (ii) attempting to move it to its neighbouring site chosen randomly, (iii) redistributing the charges among the neighbouring occupied sites and (iv) updating the amount of charge released and absorbed is repeated again and again until a desired number of steps is reached. Up to a million steps are used in this simulation.

The simulation is performed on various lattice sizes and at several concentrations p of the occupied sites in each of the lattice. Strips with various aspect ratios L_x/L_y ($=1-15$) are chosen to see the effects observed in a previous simulation [6]. We must emphasise that the charge transfer takes place here only via nearest-neighbour charge exchange and this feature is different from the simulation of Kerstein and Pandey [6] where charge exchange takes place with all the particles in the transient cluster instantaneously. There are two transport processes: (i) the particle transport accompanied by (ii) the charge exchange. The local charge spread via nearest-neighbour particles introduces a time delay or relaxation time for the charge transport in a cluster where, as in [6], this relaxation was instantaneous. The charge transfer, from source to sink, through the transient network of the particles, eventually equilibrates to a steady state in which the charge released per unit time from the source is equal to the charge absorbed per unit time at the sink. From the construction of this model, it appears that it may take a longer time for the charge distribution to equilibrate here than that found in [6]. The spatial charge distribution is observed to be more homogeneous in the present model (see the histogram presented in figure 1). Moreover, this model is computationally more efficient and at least six times faster on a scalar machine than the model of [6].

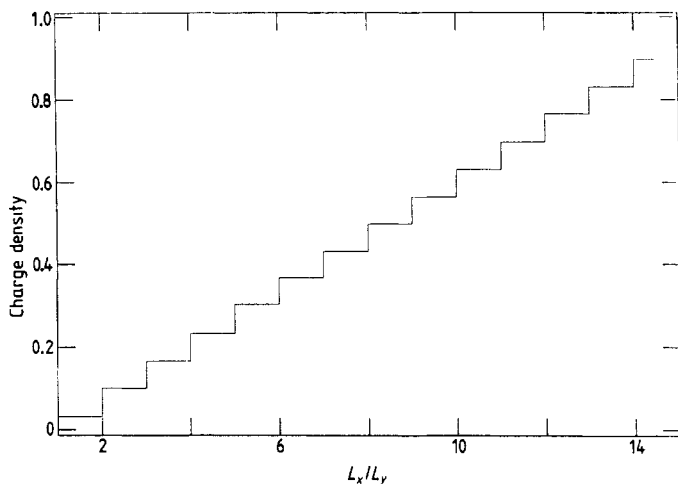


Figure 1. Charge density averaged over each square of size L_x, L_y , plotted against the aspect ratio L_x/L_y , for the sample 225×15 at concentration $p = 0.59$ at time 5×10^5 .

A plot of the total charge released from the source and the total charge absorbed at the sink against time is shown in figure 2. Such a smooth steady state achieved in this model with a constant charge density gradient assures the reliability of the data (see below). We know that, in the steady state, the conductivity σ is proportional to $j/\delta\rho$ where the charge density gradient $\delta\rho$ equals $1/L_x$ and the charge flux or the current density j is $Q/L_y t$, where Q is the charge transfer in time t . This gives us $Q \sim \sigma_e t$ with $\sigma_e = \sigma(L_y/L_x)$. Thus, from the slope of the Q against t plot, we can evaluate σ_e and therefore σ . We have calculated the conductivity this way at several concentrations for various lattices and a plot of its variation with concentration p is presented in figure 3. Clearly, the conductivity increases on increasing the concentration p from zero, but above a characteristic concentration $p \sim 0.64$ it starts decreasing. Such a non-monotonic dependence of conductivity on the concentration of the occupied

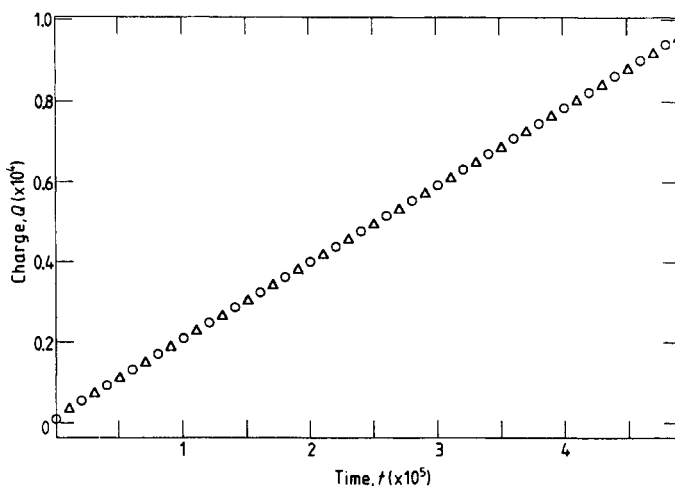


Figure 2. Total charge released from the source (Δ) and the total charge absorbed at the sink (\circ) plotted against time for the sample 225×15 at concentration $p = 0.59$.

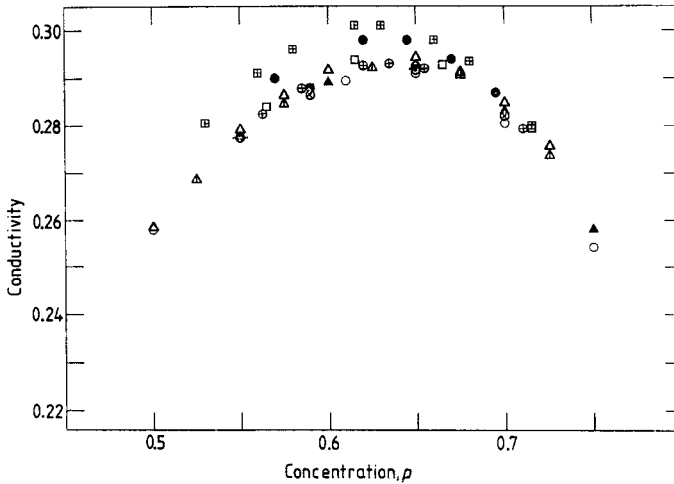


Figure 3. Conductivity σ plotted against concentration p for lattices of different aspect ratios 15 (75×5 (O)), 105×7 (\otimes), 150×10 ($-O-$), 225×15 (\blacksquare); 10 (50×5 (\boxplus)), 70×7 (\bullet), 120×12 (\blacktriangle), 5 (75×15 (\boxplus)) and 1 (20×20 (\triangle), 30×30 (\square), 60×60 (\oplus)).

sites is observed for the first time (as far as we know) in the computer simulations for stirred systems and it is worth examining this effect here. We must point out that the percolation thresholds for the onset of the infinite links along the x and y directions of the strip are different and depend upon the aspect ratio L_x/L_y [12]. However, the observed maxima in the conductivity at about $p \sim 0.64$ is considerably higher [12] than the percolation threshold for the square lattice $p_c = 0.59$. Moreover, we observe that data from all lattice sizes are collapsed almost on the same curve. This shows that the non-monotonic effect on the conductivity as a function of concentration of the conducting particles is independent of the finite size and that the maximum is not a critical divergence in the statistical limit of infinite system size.

The conducting particles are crucial in carrying the charges from the source and delivering them to the sink via nearest-neighbour hopping and charge exchange. Obviously there will be no charge transport in the absence of these particles. For the model considered here, the amount of charge transfer per unit time is proportional to the number of successful attempts to hop per unit time step (as mentioned earlier, a unit time step is defined as the time for which each particle, on average, has attempted a nearest-neighbour move). At small concentrations p of the occupied sites (i.e. A particles), there are ample vacant sites available for the jump and therefore the number of successful hops n_s is proportional to the number of particles, as most of the particles have high probability for nearest-neighbour hopping. Increasing the concentration p reduces the concentration of vacancies which decreases the number of successful jumps; the presence of A particles itself acts as a barrier for transport of these particles. For p above the characteristic concentration $p \sim 0.64$, the number of successful jumps is limited to the number of vacancies $N_b = N - N_a$ which decreases on increasing p and this reduces the charge transfer per unit time, i.e. the conductivity. A similar explanation was given in a different context for interacting diffusion on a quenched percolating lattice [11]. A precise description beyond these qualitative arguments for the dependence of the conductivity on the concentration p of the conducting particles and the appearance of maxima is highly desirable. We hope this letter will stimulate interest towards establishing such a relation.

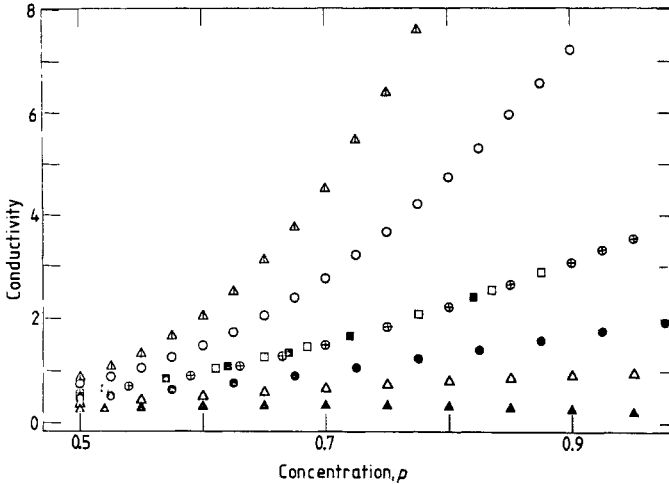


Figure 4. Conductivity plotted against concentration p for various f , the frequency of charge transfer, which is defined as the number of attempts to exchange the charges after each hopping attempt of the conducting particles. The lattice 75×5 is used for times up to 5×10^6 steps at the following frequencies: $f = 0.1$ (▲), 0.5 (△), 1.0 (●), 2.0 (⊕), 5.0 (□) and 10.0 (◆). At $f = 2.0$ lattices 105×7 (■) and 120×12 (□) are used for time steps up to 5×10^5 and 3×10^5 , respectively, to check the finite-size effect.

Data for the conductivity at higher frequency of the charge transfer indicate that the conductivity increases with concentration p of the conducting particles (see figure 4). The slope of conductivity against concentration p seems to depend strongly on the frequency of charge transfer. A non-universal power law dependence of conductivity on concentration p and the frequency of charge transfer is evident from figure 4, a detailed study of which will be published elsewhere.

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