SCALING OF DIFFUSION IN A STATISTICAL MECHANICAL MODEL REPRESENTATIVE OF SUPERCRITICAL MICROEMULSIONS

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In our presentation we will discuss the problem of electrical conduction through supercritical microemulsions, expostulating upon various computer simulation and theoretical results from our group's recent research into this problem. We will describe how the Ising model paradigm is used to generate structure dynamics that represent the microscopic dynamic behavior of the supercritical fluid microemulsion mixtures.

Our simulation results show that the approach taken yields critical exponents, for the solute transport coefficients, that are consistent with the only other published simulation that we are aware of. In addition, we find good agreement with experimental data for conductivity coefficients taken in supercritical microemulsions near their percolation transition. We also present a general scaling analysis for this system which appears to capture universal behavior, both at the random percolation limit as well as at finite Temperatures.

The talk will attempt to show that this computational/theoretical approach has the potential for being very useful for studying fundamental phenomena related to engineering problems involving transport in systems showing nanoscale dynamic disorder.

INTRODUCTION

We study the problem of diffusion through network structures exhibiting dynamic disorder, using the Ising model paradigm to generate evolving network configurations. Diffusion is studied using blind random walkers (RW). Furthermore, we partitioned the net displacement of the RWs throughout the network into two terms. These represent the contributions of transport through neighboring conducting sites and the self-diffusion of the site itself on which the RW finds itself at any given point in time.

SIMULATION APPROACH

Dynamic network structures were found with kinetic Monte Carlo (KMC) simulations, consistent with Kawasaki dynamics (i.e. constant conducting-site density) [1,2,3,4], on Ising lattice models [4,5] . At any point during the simulations conducting-site pathways (with density ϕ) are taken to be given by the network of *up* spins, using the Ising terminology, with the non-conducting-sites represented by the *down* spins. The thermodynamic properties of this system are well established in terms of the reduced Ising lattice temperature $\frac{T}{T_c}$, where T is the system temperature and in 2d, for example, $T_c = \frac{\Gamma}{0.44k_B}$ is the critical temperature in which k_B is Boltzmann's constant and Γ the spin (site)-spin (site) coupling parameter [6,7] .

Given a lattice of size $L \times L$ we pre-equilibrate the system by doing a number of Monte Carlo Steps (MCS), where a MCS consists of a complete sweep of spin exchanges, i.e. L^2 updates. In addition to the ‘’usual’’ Ising parameters another feature of our simulation model is the ability to update only a fraction of the conducting sites during any step of the simulation.

After pre-equilibration we perform the diffusion simulations as follows: a RW is placed on a randomly selected conducting site and one of its neighboring sites selected randomly. If the selected site is a conducting site the RW moves to it otherwise the RW remains fixed at its current position. The number of RW stepsattempted between consecutive structure updates is defined by the symbol n_w and the fraction of conducting sites updated per lattice sweep by q. Thus, the number of conducting sites updated each lattice sweep is $N_R = qL^2\phi$. Furthermore, we define characteristic time constants for the RW and structure evolution dynamics by the variables τ_w and T_R respectively. It follows in straightforward fashion that $T_R \sim q^{-1}$ and $\tau_w \sim n_w^{-1}$ with n_w normalized to the value one. Therefore, $T_R(q)$ represents the relative time scales of structure and RW dynamics.

RESULTS

We studied diffusion in various networks starting with a system at the random percolation limit. Some results are presented in figure 1

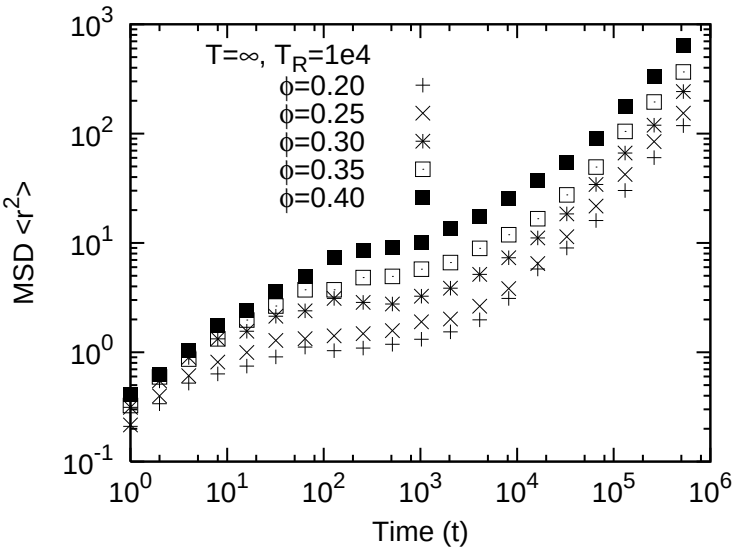

Figure 1 Diffusion behavior in the network

The results in figure 1 show three distinctive modalities: at short, intermediate and asymptotically long times. At short times we observe an increase in diffusion that quickly leads to a plateau region, during which time significant diffusion slow-down occurs where the RW appears to be trapped within its initial cluster, a phenomenon we refer to as cage trapping.

The overall diffusion behavior seen in these figures is suggestive of a system in which a scaling analysis might play a useful role in collapsing the simulation data into a "universal" curve and in figure 2 we show results using the scaling equations given by Chen et al. [8]. The scaling results seem to capture the physics of diffusion in this system in a satisfactory way.

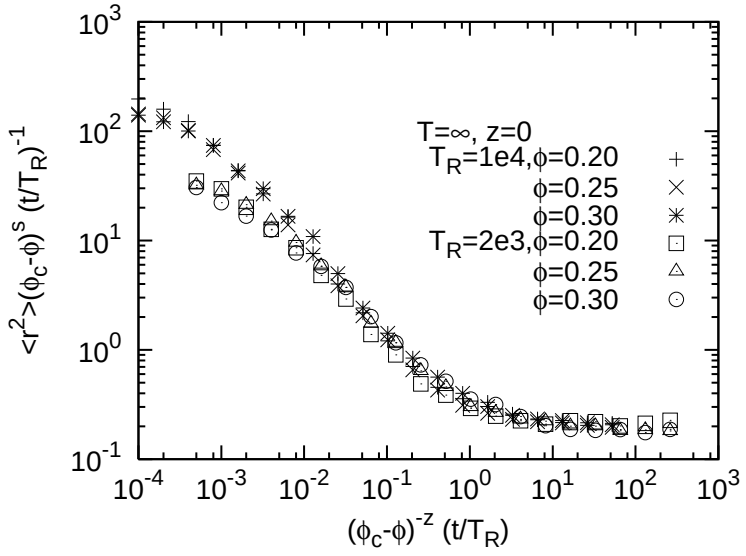

Figure 2 Scaling results for diffusion in the network.

CONCLUSIONS

Our simulation model shows a rich variety of novel diffusion behavior showing three distinctive diffusion regions: short, intermediate and asymptotically long- time transport regimes. Based upon these observations we used previously postulated scaling functions for diffusion in this system which appeared to universalize the behavior, at both the random percolation limit as well as at finite temperatures (the correlated problem). This first study suggest that the computer model presented here shows potential for being very useful for studying basic phenomena related to diffusion in correlated network structures like ion transport through supercritical microemulsions.

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