Monte Carlo simulation of anomalous transit-time dispersion of amorphous solids*

M. Silver and Leon Cohen†
Department of Physics and Astronomy, University of North Carolina, Chapel Hill, North Carolina 27514
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Simple Monte Carlo multiple-trapping model simulations of the observed anomalous transit-time dispersion have been made. The model employs multiple trapping from an exponential distribution. Our results simulate the features of the experimental observations as well as provide a rational explanation for the transition from nondispersive to dispersive transients as a function of temperature. Comparisons with recent results in *a*-Se show excellent agreement.

Scher and Montroll[1] have developed a stochastic transport model to explain the anomalous transport properties displayed by transient photocurrents in a large number of inorganic and organic amorphous materials. Their time dependence was governed by an expected hop time distribution function of the form $\psi(t) \sim t^{-(1+\alpha)}$. We have found that one can simulate the same behavior from a multiple-trapping model. By multiple trapping we mean that there are many trapping events and that the motion between traps is nondispersive diffusive motion with a superimposed drift velocity equal to μE. Our model differs from the usual single-level trapping case in that we assume an exponential distribution for the traps. This yields a power law for the probability per unit time that traps will empty. This is in contrast to the usual exponential emptying time for a single level. However, as is usual for nondispersive motion we do use an exponential law for the probability that a free carrier will be trapped. Specifically we use an exponential distribution of traps and $\psi_\tau(t) \sim e^{-t/\tau}$ for the trap-filling probability.

Comparisons between these simulation results and the Scher-Montroll hopping-time model suggest that analyses of simple transient measurements cannot by themselves distinguish between them although temperature dependences[2] as exhibited in amorphous selenium seem to be more easily explained by our multiple-trapping model.

The basic details of this type of Monte Carlo simulation calculation were previously presented by Silver, Dy, and Huang[3] in an attempt to explain the experimental results from multiple trapping and delayed release of carriers from the surface. These previous simulations did not exhibit "universality"[1] because only a limited number of trap distributions were considered. In the present calculation we do not include the complications introduced by possible delayed surface release times.

The specific time for a carrier trapping event is chosen from

$$-t_{\tau_i} = \tau_i \ln(1-r) , \tag{1}$$

where τ_i is equal to $(v n_i \sigma_i)^{-1}$, r is a random number obtained from a uniform distribution between 0 and 1, and v is the random velocity of the free carrier. The specific time to empty from this ith trap is given by a similar expression

$$t'_{ei} = -\tau_{ei} \ln(1-r'), \tag{2}$$

where as usual, $\tau_{ei} = \tau_{0i} e^{E_i/kT_L}$ and T_L is the temperature.

The assumed exponential distribution of traps is of the form $n_T \propto e^{-(E-E_T)/kT_c}$, where E_T is the highest trap level, E is measured down from the band or mobility edge, T_c characterizes the exponent of the distribution, and there are no trapping levels between 0 and E_T. While it is not at all essential, we assume that the cross section of the traps is independent of energy so that the probability that a trap is filled depends only on the density.

We use the expectation values for the trapping time and the trap emptying time for the entire distribution rather than consider each level separately as was done previously.[3] This technique is satisfactory as long as the number of particles is large. Since the trapping follows nondispersive diffusive motion between trapping events, the expectation value for trapping time is

$$\tau = \left(v\sigma \int_{E_T}^{\infty} n_T(E)\, dE \right)^{-1} ,$$

where v is the random velocity at the band or mobility edge and σ is the cross section of the traps. This leads to a trapping time for any specific event to be governed by

$$t_\tau = -\tau \ln(1-r) . \tag{3}$$

The expectation value for the trap emptying time is gotten from

$$\psi_e(t) = \frac{1}{kT_c} \int_{E_T}^{\infty} \exp(-t\nu_0 e^{-E/kT_L}) \nu_0 e^{-E/kT} e^{-E/kT_c}\, dE , \tag{4}$$

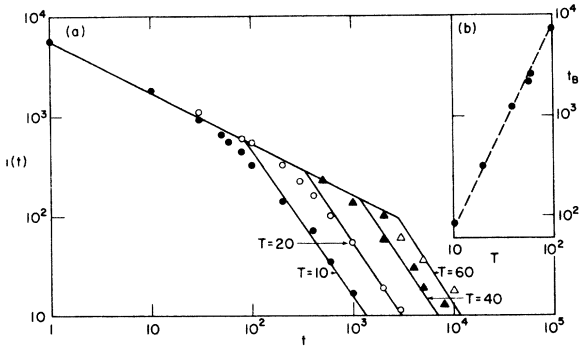

FIG. 1. (a) Log-log plot of the simulated current vs time for various values of the free-carrier transit time T. These simulations were obtained for 10^4 particles, $t_0=1$, $\tau=1$ and $\alpha=0.5$. The intercept between the two regions where the slopes are $-\frac{1}{2}$ and $-\frac{3}{2}$ $[(\alpha-1)$ and $-(\alpha+1)]$ is designated as the time t_B. Some of the calculated points are shown to indicate the actual trend. (b) Log-log plot of t_B vs T. The values of t_B were taken from (a). The slope of this curve is $1/\alpha=2$.

where T_L is the temperature, $\nu_0=N_c\sigma v$, and N_c is the density of states at the mobility or band edge. For simplicity we have used

$$\psi_e(t)=\alpha t_0^{\alpha}/(t_0+t)^{1+\alpha}\ , \tag{5}$$

which retains the basic character of Eq. (4); $\alpha=T_L/T_c$ and $t_0=(1/\nu_0)e^{E_T/kT_L}$ for $E_T\gg kT_L$. In terms of the random numbers, this distribution ψ_e yields a time for any specific emptying event given by

$$t_e=t_0[\,1/(1-r)^{1/\alpha}-1]\ , \tag{6}$$

where again r is one of the random numbers between 0 and 1.

To obtain a simulation of the current we used between 10^4 and 5×10^4 particles and watched their progress through the material until $\sum t_\tau=T$, where T is the nondispersive free transit time of the carriers. At any time t one determines the current by counting the number of particles which are not in traps.

For these simulations, we have at our disposal four parameters T, τ, t_0, and α. Figure 1 shows $\log_{10}i$ vs $\log_{10}t$ for various free transit times T. As can be seen, the results break up into two regions where the slopes of the curves are approximately $(\alpha-1)$ and $-(\alpha+1)$ as obtained by Scher and Montroll.[1] It is obvious that a plot of $\log_{10}(i/i_B)$ vs $\log_{10}(t/t_B)$ would show a universal curve. Further, as seen in the inset in Fig. 1, there is nonlinear dependence of the break time between the two regions as a function of the free transit time T. Thus, we also obtain the strange results that the apparent mobility, depends upon thickness and field ($\mu_a=L/t_BF$). It should be emphasized that in this model, there is a real time-independent mobility for the free carriers.

Another interesting result is obtained if one keeps T and α constant but varies t_0. This simulation is perhaps what one might expect by changing the temperature[4]; i.e., $t_0=(1/\nu_0)e^{+E_T/kT}$. [Variation of T through the mobility is not included for simplicity. Variation of α with temperature was also excluded because the shape of the $i(t)$-vs-t curves are very insensitive to α in the region $0.7<\alpha<1$. For reasons given below we used a value of $\alpha=0.7$.] These simulations are shown in Fig. 2. As can be seen, the break time decreases as t_0 decreases (T_L increases) giving an activation energy for the apparent mobility. In addition the shape of the curves also change. For $t_0\ll\tau$ the simulations give non dispersive transient currents as expected. The slopes of the curves are no longer $\alpha-1$ and $\alpha+1$. For our condition, only for $t_0\geq0.8$ do we obtain dispersive curves as indicated in Fig. 1. One can understand this behavior from the following: in order for the trapping to hold up the motion of the carriers, the emptying time for any event must be comparable to the trapping time. The number of trapping events is approximately T/τ. Now to get an emptying time $t_e>\tau$ for $\alpha=0.7$ requires a random number

$$r>1-[\tau/t_0+1)^{\alpha}]^{-1}\ .$$

For example, in our simulation $T/\tau=10$ and when $t_0=\frac{1}{10}\tau$ then $r>0.81$. This means that only about two out of the ten trapping events will significantly slow down the motion of the carriers and there is little dispersion. On the other hand if $t_0=0.8\tau$ then $r>0.43$ or five or six out of the ten trapping events will significantly slow down the motion of the carrier and one would observe dispersion. Consequently, an experimental test of this model

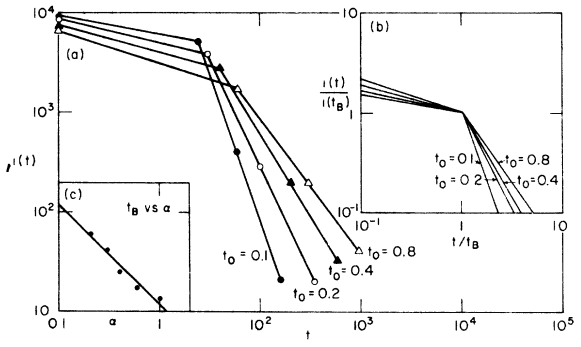

FIG. 2. (a) Log-log plot of current vs time for various values t_0. The value used for α was 0.7 so that currents would approximate results of Pfister. (b) Log-log plot of normalized current vs normalized time. Data was obtained from curves in (a). (c) Log-log plot of t_B vs α. The other parameters are $T=10$, $t_0=0.5$ and $\tau=1$.

would be to look at the dispersion as a function of the free-carrier transit time. As one lowered the field or increased the thickness one should observe a transition from nondispersive to dispersive transients.

Our simulations may be compared with those observed experimentally by Pfister[2] for amorphous selenium. We show normalized current time curves in Fig. 2 for better comparison with Pfister's results. If our model is a reasonable representation of the experimental results in selenium, the observed differences between high temperatures and low temperatures,[4] can be simply attributed to multiple-trapping parameters rather than solely due to changes in the disorder parameter α as proposed by Pfister.[2] As Pfister points out, no theoretical framework existed to analyze $i(t)$ at higher temperatures, because the experimental results in this regime did not generate a universal curve. Our model does not predict a universal curve at high temperature and is therefore consistent with his experimental results.

Finally, we also show in Fig. 2, the simulations for various α's for large t_0's and a given T (dispersive regime). In all cases used, the sum of the slopes of the two regions (before and after the break point) add up to -2. The break time is proportional to $T^{1/\alpha}$ similar to what was obtained by Scher and Montroll.[1] It was from these simulations that we found that the slopes of $i(t)$ curves were insensitive to α for $0.7 < \alpha < 1$.

In this comment, we have tried to show that multiple trapping can give dispersive transients and that hopping was not a essential feature. Further, the multiple-trapping model easily lends itself to explaining the transition from nondispersive to dispersive transients as a function of temperature providing $E_T \gg kT$. We will continue this work using exact trap emptying probabilities to try and find some other distinguishing features between multiple-trap emptying and a dispersive hopping-time model.

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[1]H. Scher and E. W. Montroll, Phys. Rev. B 12, 2455 (1975).

[2]G. Pfister, Phys. Rev. Lett. 36, 271 (1976).

[3]M. Silver, K. S. Dy and D. L. Huang, J. Non-Cryst. Solids 8-10, 773 (1972).

[4]According to our model, the transit-time activation energy would be given by E_T except at very high temperatures where the mobility would tend to saturate. If one observes a transition from dispersive to nondispersive transients with temperature but no tendency to saturate, then there may be two possible reasons: (i) one has not quite reached the saturation temperature (experiments at still higher temperatures will determine the validity of this idea) and (ii) there is a relatively-low-density single-level trap of energy E_D, where $E_D \gg E_T$. E_D would then determine the activation energy since from detailed balance, one has approximately $\mu_a \propto (L/t_B F)e^{-E_D/kT_L}$.