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A simulation of the multiple trapping model for continuous time random walk transport

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A multiple trapping model is used to study the dispersive transport of holes in insulators. The one-dimensional Poisson and continuity equations are solved numerically along with the trap rate equations that model multiple trapping. The transient current due to a pulse of radiation is obtained as a function of the spread in the trap energy levels and the trap density distribution. The main properties of continuous time random walk transport, namely universality and superlinear dependence of the transit time on the electric field and oxide thickness, are verified.

I. INTRODUCTION

One of the features that marks disordered solids like the chalcogenide glasses and silicon dioxide is the dispersive nature of carrier transport. Mathematically, dispersive transport is modeled by the continuous time random walk (CTRW) formalism of Scher and Montroll.[1,2] They have shown that a good fit to experimental data is obtained if one assumes a distribution function for event times, $\psi(t)$, which decays slowly with time, as for example a power law in time. The function that they have chosen is $t^{-(1+\alpha)}$, where α is called the disorder parameter and takes on a value between 0 and 1.

The principal problem in CTRW transport is to find a form for $\psi(t)$ based on the underlying physical mechanism of transport. Pfister and Scher[3] have shown that both hopping and multiple trapping with a trap density that decreases exponentially with energy, give rise to a power law distribution function with one difference, namely, hopping gives rise to transient currents that are universal with respect to temperature but multiple trapping does not. Transient hole currents in silicon dioxide turn out to be universal with respect to temperature indicating a hopping mechanism. Transport in silicon dioxide is believed to occur via the formation and hopping of small polarons.[4–7] In the case of a-Se and As_2Se_3, although experimental evidence seems in favor of multiple trapping, small polaron hopping is not completely ruled out.

Simulation and modeling of radiation effects as well as hot-carrier degradation effects in metal-oxide-semiconductor (MOS) structures require an accurate model for hole transport, preferably one that will fit into the conventional device simulation framework consisting of the Poisson and continuity equations. To model hopping transport, the CTRW framework will have to be used, which still contains fitting parameters to describe the electric field dependence of transport. As a result, it becomes difficult to take into account spatially varying electric fields in the oxide that occur due to the trapping of holes into deep traps in the oxide. Multiple trapping, on the other hand, is described completely by a set of differential equations consisting of the Poisson, continuity, and trap rate equations and can be more readily used for simulating various degradation effects. As long as the temperature is not varied, multiple trapping can be used as a mathematical model to give accurate results for silicon dioxide.

Schmidlin[8] and Noolandi[9] have analytically solved the differential equations, but have made several approximations. Monte Carlo simulations of multiple trapping have been done by Silver and Cohen[10] for As_2Se_3. They have assumed a spatially uniform trap density that decreases exponentially with energy, with capture times constant and emission times an empirical function of α, the disorder parameter. Curtis and Srour[11] have numerically solved a set of trap rate equations along with a rate equation for decrease of holes in the valence band. However, they have some fitting parameters which they use to fit their results to experimental data.

None of the above models are in a form where they can be used directly in a simulator. Moreover, all of them make some approximations in order to arrive at the solution. We have done a numerical simulation of dispersive transport via multiple trapping, by solving the Poisson and continuity equations along with a multiple trapping model. In this paper we present the results of this simulation.

II. THE MODEL FOR MULTIPLE TRAPPING

Figure 1 shows a typical plot of the transient current as a function of time that is expected from the CTRW model. It is seen to consist of two distinct portions. The initial slope of the current transient is $-(1-\alpha)$ and at very large times, the slope is $-(1+\alpha)$ on a log-log plot, α being the disorder parameter. The intersection of the lines defined by these two slopes is by definition the transit time.

As mentioned previously, a trap density that decreases exponentially with energy results in CTRW transport. This is for the following reason. If the distribution of trap energies is exponential, it means that there are a large number of shallow traps that capture and reemit holes several times within a transit time. This gives rise to a large spread in the free-carrier distribution and the centroid of free holes moves at a much slower rate. Besides, there should also be a significant number of deep traps (i.e., traps that emit carriers at times larger than the transit times) in order to ensure the slow decay of current after the transit time. The universality of the current shape implies that irrespective

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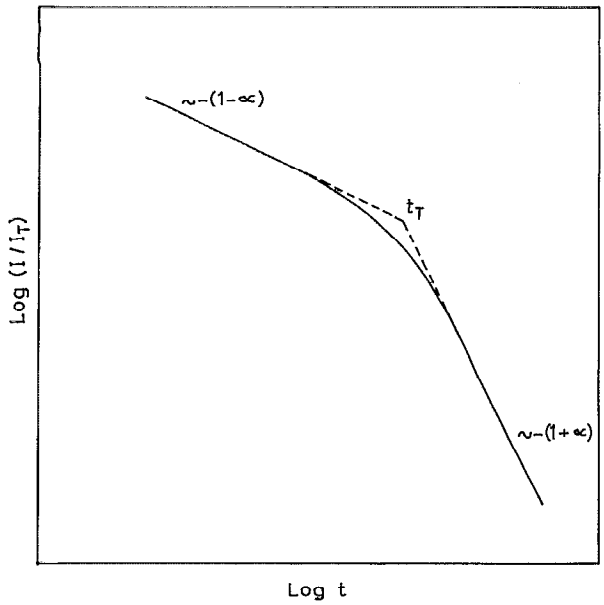

FIG. 1. Typical transient current obtained expected from the CTRW model.

of the transit time, there are always some traps with emission times that are much larger than the transit time, i.e., there is a wide spread in the trap energies.

In our model, we have a single trap energy level at each grid point, with the trap energies or the emission times varying randomly from point to point. From the discussion above, it is clear that the trap energies cannot have a uniform distribution. We have generated trap energies with an exponential distribution. Typically, the emission times vary from a few nanoseconds to a few tens of seconds.

Theoretically it is impossible to prove that this model gives rise to CTRW transport. But the model seems physically reasonable and should give correct results in a three-dimensional simulation. For simulation in one dimension however, this model is an approximation since it assumes symmetry in two spatial directions.

The exponential distribution of traps were generated using the inverse CDF (cumulative distribution function) technique,[12] which leads to trap energies given by

$$E_T=-\frac{1}{c}\ln(1-\gamma),$$

where c is the coefficient of the exponent in the exponential distribution and γ is a random number that is uniformly distributed between 0 and 1. The corresponding emission times are therefore

$$\tau_e=\frac{1}{\sigma_p v_{\rm th} N_v}e^{E_T/kt},$$

where σ_p is the capture cross section assumed to be constant, $v_{\rm th}$ is the thermal velocity, and N_v is the density of states in the silicon dioxide valence band. We have assumed a value of $\sigma_p=10^{-16}$ cm^2, $N_v=10^{19}$/cm^3, and $v_{\rm th}=10^7$ cm/s. None of these parameters have really been determined for silicon dioxide, but the exact values of these parameters are not very important. What matters in CTRW transport is the distribution of emission times, and changes in these parameters would only mean that the position of the energy levels must be changed slightly to give similar values of the emission times.

Trapping and detrapping at each point is modeled using first-order trapping kinetics. In order to obtain the transient current, the following set of equations needs to be solved in the oxide:

$$\frac{d^2\psi}{dx^2}=-\frac{q}{\epsilon_{\rm ox}}(p+p_t-n),$$

$$\frac{\partial p}{\partial t}=-\frac{1}{q}\frac{dJ_p}{dx}+G_{\rm ox}-\frac{dp_t}{dt},$$

$$\frac{\partial n}{\partial t}=\frac{1}{q}\frac{dJ_n}{dx}+G_{\rm ox},$$

$$\frac{dp_t}{dt}=\sigma_p v_{\rm th} p(N_{\rm tp}-p_t)-\frac{p_t}{\tau_e},$$

where

$$J_p=qp\mu_p E-qD_p\frac{\partial p}{\partial x},$$

$$J_n=qn\mu_n E+qD_n\frac{\partial n}{\partial x}.$$

In the above equations, ψ, n, and p are the electrostatic potential, electron, and hole densities respectively and p_t is the trapped hole density. $G_{\rm ox}$ is the generation rate in the oxide assumed to be due to a pulse of radiation, μ_n and μ_p are the electron and hole mobilities in the oxide, $N_{\rm tp}$ is the trap density at each point, and τ_e are the random emission times of these traps.

In order to obtain the solutions in a MOS capacitor, the poisson and continuity equations also need to be solved in the semiconductor. The numerical techniques used as well as the boundary and interface conditions have been discussed in a previous paper.[13]

The measured hole current per unit area can be calculated as

$$I_p=q\langle p\rangle v_D,$$

where

$$v_D=\frac{dx_0}{dt}.$$

In the above equation, x_0 is the centroid of the free-charge distribution and $\langle p\rangle$ is the average number of holes in the valence band given by

$$\langle p\rangle=\frac{1}{t_{\rm ox}}\int_0^{t_{\rm ox}} p\,dx.$$

The velocity of the centroid is calculated numerically by finding the position of the centroid at each time point. This is essentially the average conduction current per unit area.

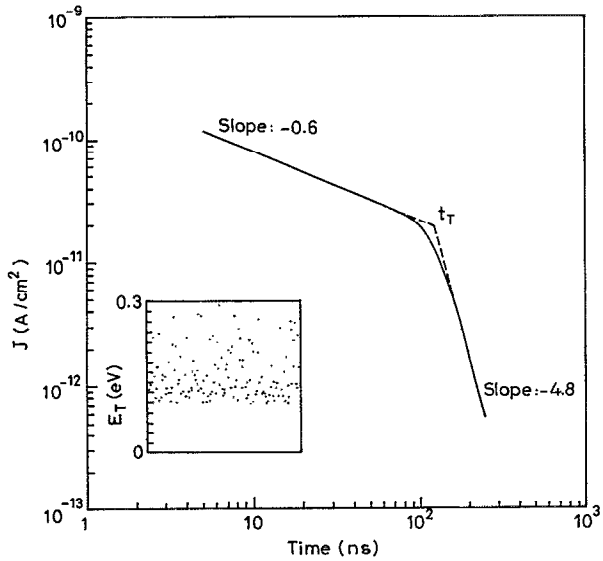

FIG. 2. Transient current obtained if the trap energies lie between 0.1 and 0.3 eV. The oxide thickness T_{ox} is 500 Å and the gate voltage V_G is 4 V.

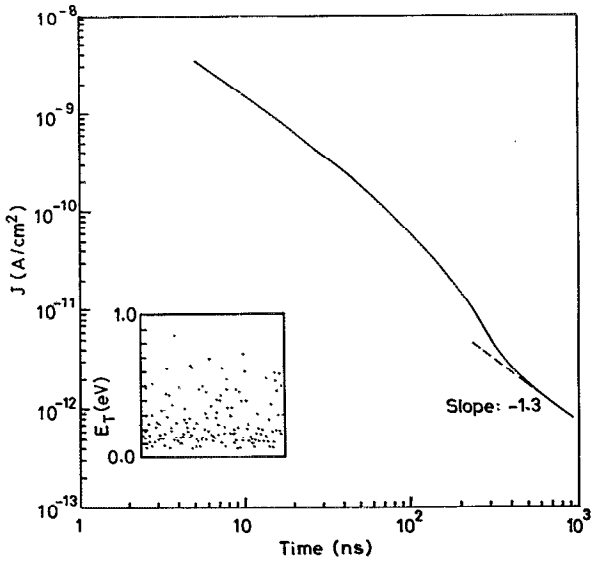

FIG. 4. Transient current obtained if the trap energies lie between 0.1 and 1.0 eV. T_{ox} is 300 Å and V_G is 2 V.

Due to the relatively large mobility of electrons in the oxide (20 $cm^2/V\,s$ as compared to 10^{-5} $cm^2/V\,s$ for holes), electrons get swept out of the oxide in a few picoseconds. Therefore, in order to obtain the transient hole current, the electron continuity equation can be neglected, which gives a set of three differential equations to be solved at each point.

III. RESULTS OF THE SIMULATION

Figures 2–4 show log-log plots of the transient hole current versus time. In each of these cases, the trap energies are assumed to lie within a particular energy range just above the valence band, i.e., an exponential distribution of trap energies is first generated and the distribution is then truncated so that all the energies lie within a specified energy range, for example 0.1–0.3 eV in Fig. 2. The trap energy distribution is shown in each of these figures as an inset. In each case the trap density is assumed to vary with the trap energy as $N_T = 5\times10^{16}\, e^{-E_T/0.5(\mathrm{eV})}$, where E_T is the trap energy. This particular distribution of trap density with energy does not have any special physical significance and variation of the transient current with different distributions of the trap density is discussed later.

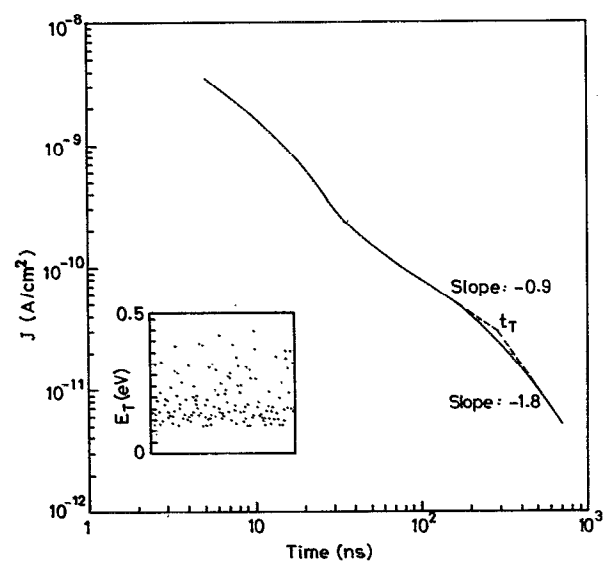

FIG. 3. Transient current obtained if the trap energies lie between 0.1 and 0.5 eV. T_{ox} is 300 Å and V_G is 2 V.

Unlike the typical transient that is obtained for CTRW transport, shown in Fig. 1, these transient currents are seen to contain an initial spike where the current decays sharply (except for the current trace in Fig. 2, which has a very low spread in the trap energies). This is not predicted in CTRW theory, but has been observed in transient currents measured in As_2Se_3 and a-Se.[3] This occurs due to the high initial trapping rates and very little emission from the traps. After this initial sharp decay, there is a more gradual decay of the current as expected from CTRW transport which goes as $-(1-\alpha)$. This occurs when the trapping rates of the deeper traps decrease and the carriers begin to get emitted from the shallower traps. Finally after the transit time, which is obtained from the intersection of the two lines as shown in the figures, the current once again decreases more rapidly as carriers are also lost to the contact.

There are two trends clearly seen in these curves. First, as the spread in the trap energy increases the initial decay continues for a much longer time. When the spread is very small and the traps are almost all shallow traps as in Fig. 2, very few carriers get trapped and even those that get trapped get reemitted very quickly. So the resulting characteristic is very near a characteristic obtained for drift-diffusion transport in extended states. When the spread becomes very large, there are a much larger number of deeper traps and hence the initial decay continues for a

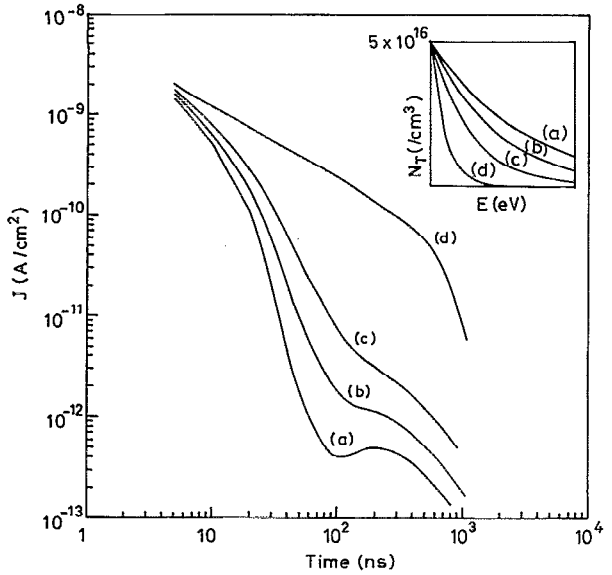

FIG. 5. Transient current for different trap density distributions. The variation of trap density with energy is (a) $e^{E_T/0.7(eV)}$, (b) $e^{E_T/0.5(eV)}$, (c) $e^{E_T/0.3(eV)}$, and (d) $e^{E_T/0.1(eV)}$.

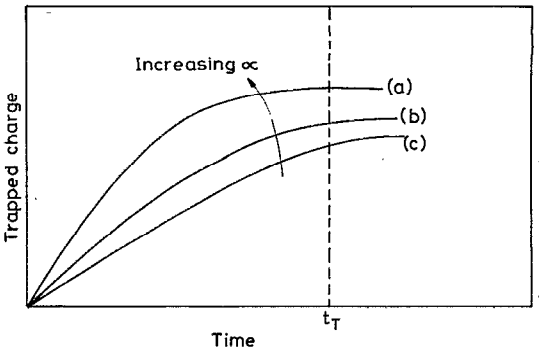

FIG. 6. Dependence of the disorder parameter α, on the trap density distribution with energy, for a larger density of deeper traps. Curves (a), (b), and (c) in this figure correspond to (a), (b), and (c) of Fig. 5.

much longer time and as seen in Fig. 4, it completely masks out the slower decay before the transit time. So in this curve, there is no clear transit time.

The second trend that can be observed is in the slope of the post-transit time decay. This slope is clearly seen to decrease as the spread in trap energies increases. This makes sense because as the spread increases, the number of deeper traps increases and more carriers get trapped in these deeper traps. Since these carriers then do not get emitted until after the transit time, the slope of the post-transit decay is more or less controlled by the emission time of the deeper traps. The larger the emission times, carriers get emitted at a much slower rate and hence the current decay is slower.

Figure 5 shows the transient current obtained for a fixed spread in the trap energies, but for different variations in the trap density with energy as indicated in the figure. Curve (a) has the maximum density of deeper traps and hence has the largest amount of initial decay. This is followed by a plateau up to the transit time, which indicates that there is not much capture or emission of carriers. (Actually there is a slight increase in the current due to emission of carriers from the shallower traps.) Curves (b) and (c) show the current traces obtained for a decreasing density of deeper traps. As the trap density decreases, the capture probability of these traps decreases, leading to an initial sharp decay followed by a more gradual decay in the current. In these two cases, holes continue to get trapped right up to the transit time and as a result, the current continues to decay until the transit time. When the density of the deeper traps decrease further, the initial sharp decay disappears altogether due to the very low capture rate and only a gradual decay is observed right from the beginning as shown in curve (d).

Using these curves, it is possible to give a physical meaning to the disorder parameter α. In materials like a-Se and As_2Se_3, there is a sharp decay in the current before the more gradual decay that goes as $t^{-(1-\alpha)}$. In this case α increases with an increasing density of deeper traps. This can be understood using Fig. 6. This figure shows the trapped charge as a function of time for different trap densities and hence different capture rates of holes. If each of the trap density distributions that we have considered were to be represented by an equivalent trap level, curve (a) in Fig. 5 would correspond to a characteristic similar to the one shown in curve (a) in Fig. 6. Here the trap density is large, leading to large initial capture rate. As a result, the free-hole density and therefore the current decreases sharply. This in turn results in a sharp decrease in the subsequent capture rate of holes by the deeper traps at other points in the oxide and thereafter hardly any holes are lost to the traps. Therefore, the current remains more or less constant up to the transit time, which according to Pfister and Scher,[3] corresponds to an α of 1. As the density of traps reduces, the initial capture rate of holes by the traps reduces and the trapped charge builds up more gradually, as seen from Fig. 6. Since now holes are lost to the traps at a much slower rate, instead of a plateau one sees a continuing decrease in the current with a slope (on a log scale) that is around $-(1-\alpha)$. Therefore, with a decreasing trap density, α decreases since then, the capture of holes is spread out over a much longer time. In all these cases, a significant number of carriers get captured, so that the post-transit decay is slow and is controlled by the emission times of these deeper traps.

When the trap density reduces to a point where the initial decay disappears completely and there is only a gradual decay right from the beginning with a slope of $-(1-\alpha)$, then α can be interpreted slightly differently. In this case the trapped charge builds up as shown in Fig. 7. Since the capture probability is quite small, holes are lost to the traps at almost a constant rate right up to the transit time. As the trap density of the deeper traps reduces, the capture rate reduces further and at any time, there is a much smaller amount of charge trapping resulting in a smaller rate of current decay and hence a larger value of α. In the limit when there are no traps, the current trace

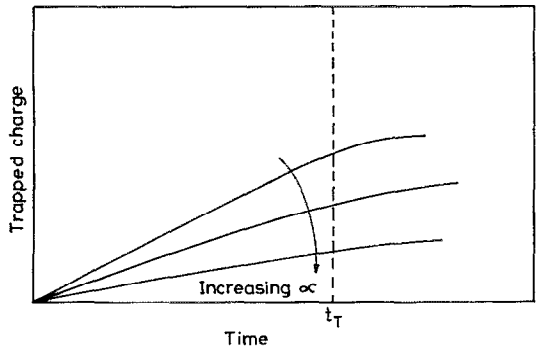

FIG. 7. Dependence of α on the trap density distribution with energy for a smaller density of deeper traps.

corresponding to drift diffusion in extended states is obtained which corresponds to an α of 1. A larger value of α would correspond to fewer carriers in deeper states and hence will have a larger post-transit time slope. Transient currents in silicon dioxide show this type of behavior. Measured values of α are quite small, between 0.1 and 0.3 (Ref. 5,14) indicating a fairly large density of deeper traps.

Since we are interested in hole currents in SiO_2 which does not show the initial sharp decay, we have used a trap density which varies with the energy as $e^{E_T/0.1(eV)}$, which does not give the initial spike. All further simulations are done with this distribution of trap density.

Figure 8 shows the transient current obtained for different values of the applied voltage. It is seen that the initial slope decreases with an increasing electric field in the oxide. This is because as the field increases, the holes get swept away faster and the capture efficiency of the traps reduces. As a result, a smaller number of holes are captured by the traps and the current decays at a slower rate. Therefore it is not possible to obtain a single value of the

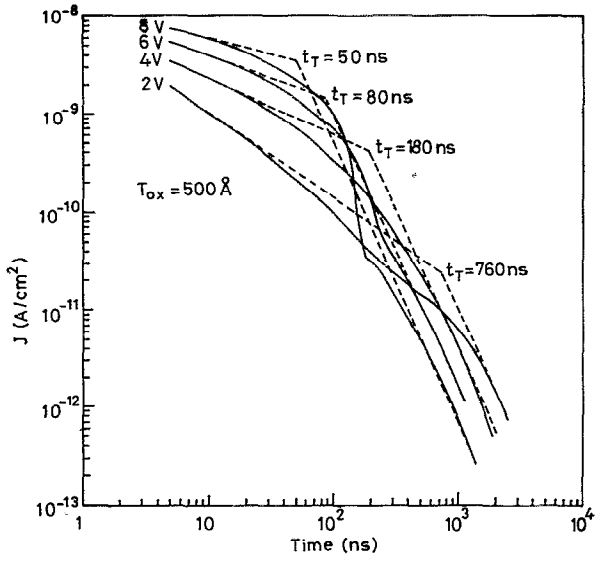

FIG. 8. Transient hole currents for different electric fields. The intersection of the dashed lines is taken as the transit time.

parameter α. This is inconsistent with the CTRW theory in which the initial slopes are parallel irrespective of the field. Obtaining parallel slopes means that the number of carriers trapped is the same irrespective of the field. One way to get this is by increasing the trap density, so that the trapping rate is very high which will result in the trapping of carriers dominating over the action of the electric field for all typically used electric fields. However in our model, increase in the trap density results in the presence of an initial spike which is not seen in SiO_2. The other way is to have traps of several energy levels at each grid point, so that the amount of trapped charge is high. But the capture rate of each of the trap levels can be kept small, so that there is only a gradual decay of current right upto the transit time without an initial spike. This is what is seen in the simulation done by Silver and Cohen.[6] This is a limitation of our model, because once a trap at a particular grid point reaches steady state, there is no further trapping at that point.

However, as seen from the figure, the final slopes are approximately parallel which makes sense as this slope should be determined by just the emission rates of the traps. But the slope is larger than expected from the CTRW theory [around -2.2 instead of $-(1+\alpha)$]. This indicates that not enough carriers are trapped in the deeper traps. One way to increase the trapped charge without increasing the initial trapping rates considerably, is to have several trap energy levels at each point so that none of the traps reach steady state before the transit time but a large amount of charge is trapped. This is an indication that for simulations of CTRW transport using multiple trapping in one dimension, multiple trap energy levels at each grid point are necessary.

Although not very apparent from Fig. 8, the post-transit time slope keeps on increasing with increasing time. This also seems to be the case in some of the published experimental results of transient currents in a-Se and As_2Se_3,[2,3] but not in SiO_2.[5] This increase in slope is consistent with our model. In the initial stages, after the transit time, there is still both capture and emission of carriers. But as more and more holes are lost to the contact, the trapping rate reduces. As a result, the effective number of carriers getting emitted keeps on increasing and therefore carriers are lost at a faster rate to the contact. This should be true irrespective of the number of trap energy levels at each grid point, although the effect will probably be smaller as the number increases.

One other effect that is noticeable in the current curves in Fig. 8 is the sharp decrease in the current near the transit time at high fields. This happens because for very short transit times, not enough charge is trapped and a considerable amount of charge is lost to the contact at a time corresponding to the transit time that would have been obtained if there was no trapping of carriers. However, the asymptotic slope is still determined by the emission time of the traps.

Figure 9 shows the transit time, determined from the intersection of the two straight lines obtained from the asymptotic slopes as shown in Fig. 8, as a function of

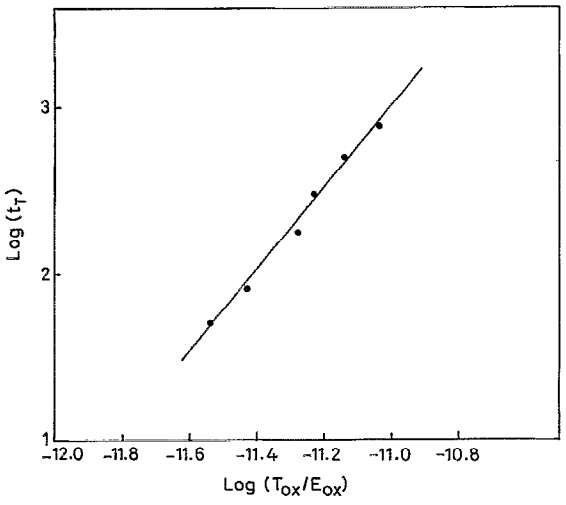

FIG. 9. The transit time as a function of T_{ox}/E_{ox} on a log-log plot. The inverse of the slope is α.

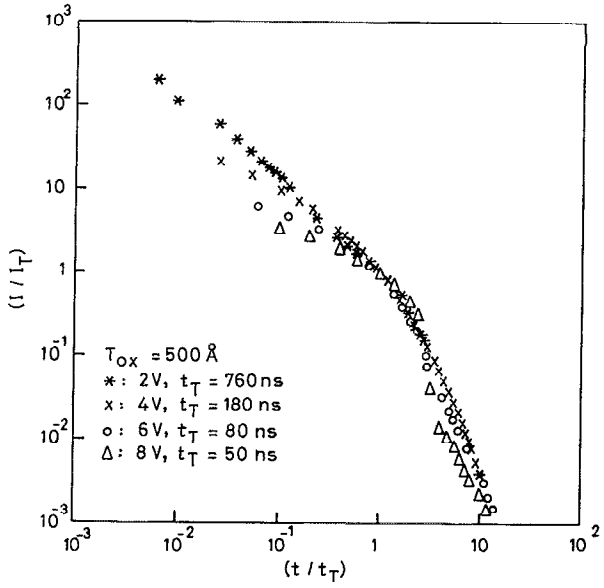

FIG. 10. The normalized hole currents for different electric fields. The oxide thickness is 500 Å. Time is scaled to the value of the transit time obtained from Fig. 8 and the current is normalized to its value at the transit time.

(T_{ox}/E), where T_{ox} is the oxide thickness and E is the electric field in the oxide. According to the CTRW theory, the transit time varies superlinearly with both the electric field and the oxide thickness, with a variation that is approximately given by $(T_{ox}/E)^{1/\alpha}$.[2] Using this relationship, we obtain an α of about 0.4, which is the average value of α determined from the pretransit time slopes. It is not surprising that the transit time depends superlinearly on the oxide thickness and the electric field. As the oxide thickness increases, the transit time increases due to two reasons. Not only do the carriers have to travel longer to reach the other boundary, but they also get trapped more often and this results in the superlinear dependence. Similarly, with an increase in the electric field, not only does the transit time decrease due to an increase in the drift velocity, but the capture efficiency of the traps also decreases which means that on an average, the carrier spends a smaller amount of time in the trapped state further decreasing the transit time. Also it makes sense that the exponent depends on α, since α essentially is a measure of the capture efficiency of the traps.

A final and perhaps the most important property of CTRW transport is the universality of the transient current, which means that if the transient current scaled to its value at the transit time is plotted as a function of time in units of the transit time, it traces out the same curve irrespective of the electric field and the oxide thickness. In order to verify this, we have plotted the normalized current versus time on a log-log scale in Fig. 10, for different values of the applied voltage. It is seen that except for very short times (<20 ns), the transient current is universal with respect to the applied field. In these short times, probably the holes have not yet started moving dispersively according to CTRW transport. Figure 11 shows a similar plot for different oxide thicknesses and once again, the currents are seen to be approximately universal. This result is readily understandable, since as we have seen earlier, the initial slope is determined by the trap density distribution with energy (i.e., capture rate of the traps) and the final slope is controlled by the distribution of emission times of the traps. Therefore, as long as the effect of the electric field does not dominate over the effect of the traps, the currents must be universal since it is a property of the structure of the material rather than externally applied conditions.

One of the major effects of radiation incident on an MOS device is the long-term flatband voltage shifts occurring due to the trapping of radiation-generated holes in

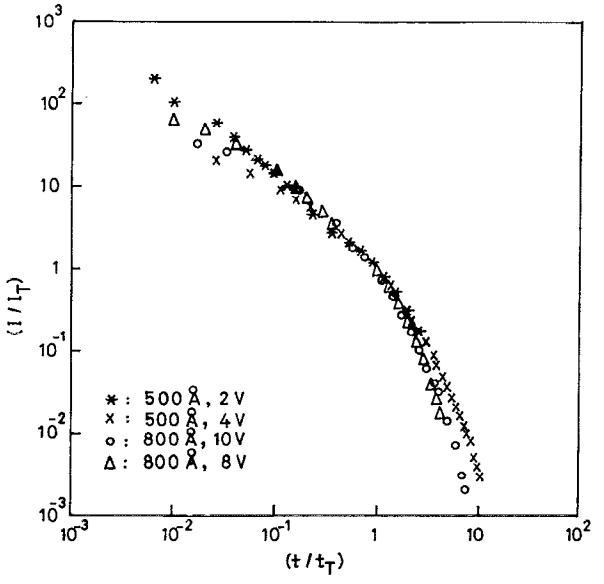

FIG. 11. The normalized hole currents for two different oxide thicknesses and different values of the applied electric fields. Time is scaled to the value of the transit time and the current is scaled to its value at the transit time.

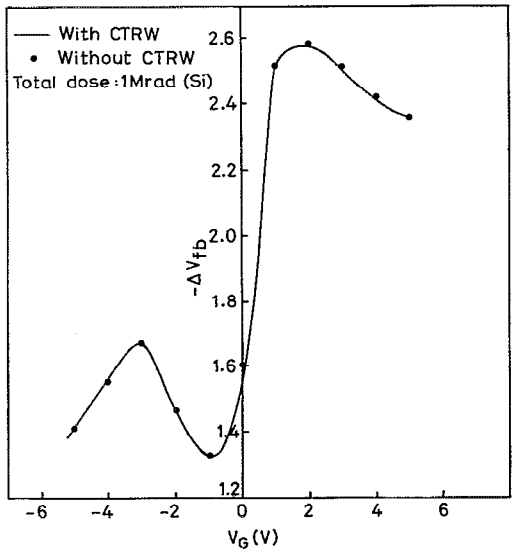

FIG. 12. The flatband voltage shifts due to trapping of holes in deep traps near the interface for a total dose of 1 Mrad(Si). The solid line is obtained using the multiple trapping model for hole transport and the points are obtained using drift diffusion in the valence band.

deep traps near the interface. (The emission times of these traps is 10^4–10^6 s.) Simulations of this process done so far have used the drift-diffusion model for hole transport.[13,15,16] We have added the multiple trapping model to the equations described previously[13] and obtained the flatband voltage shifts as a function of the applied gate bias for a total incident dose of 1 Mrad(Si). A comparison was made with the flatband voltage shifts obtained using the drift-diffusion model. Figure 12 shows the results of this comparison. It can be seen that there is no difference in the two results. This is understandable because under uniform generation of electron-hole pairs, very few holes are trapped in the shallow traps involved in hole transport, since the emission times of these traps are very low (ns to a few seconds). As a result, there is not much difference in the number of holes available for trapping into the deep traps and the trapped charge density in these traps remains almost the same. Therefore at room temperature, the fact that holes move dispersively according to the CTRW model, makes very little difference to the flatband voltage shifts due to the deep traps near the interface and it is possible to use the drift-diffusion model to obtain ΔV_{fb}. However, any sort of transient simulation as well as simulations at low temperatures or very high dose rates will need an accurate model for hole transport.

IV. CONCLUSIONS

In this paper we have studied the CTRW transport of holes in silicon dioxide using a multiple trapping model. The model is able to simulate some of the main features of CTRW transport. The transient currents show approximate universality and the transit time is seen to depend superlinearly on the electric field and oxide thickness as expected from the CTRW theory. Moreover, this simulation gives a fairly clear physical picture of dispersive transport that is not very apparent from the complex mathematical formalism of CTRW.

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