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Dispersive transport of carriers under nonuniform electric field

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We have presented in this paper a semi-numerical simulation of dispersive transport under one-dimensional nonuniform electric field which could be used to study dispersive transport of carriers in the oxide. Our simulation is based on continuous time random walk principles (CTRW). Previous formulations using CTRW were derived under the assumption of uniform electric field. Comparison of our simulation results with the equivalent uniform field case shows that the treatment of nonuniform electric field is necessary to correctly predict events linked to dispersive transport, such as the growth of trapped oxide charge due to hole trapping or interface states due to H⁺ ions reaching oxide semiconductor interface of metal-oxide-semiconductor devices. © 1995 American Institute of Physics.

I. INTRODUCTION

In recent years, the theory of dispersive transport has often been used in modeling the transport of holes¹ and H⁺ ions² through the gate oxide of metal oxide field effect transistors (MOSFET) instead of the conventional drift-diffusion equation. Dispersive transport of carriers differs significantly from the conventional transport obeying Gaussian statistics.³ In the former carriers have widely varying characteristic event times. For example, the probability of a hole hopping from one hopping site to the next might fluctuate widely due to random location of sites in the sample. These wide fluctuations in the characteristic times of hopping result in some holes getting trapped for much longer than others. The proportion of less mobile holes increases in time leading to a reduction of mobility as a function of time. This anomalous behavior of motility is distinctly different from the conventional Gaussian transport where mobility is a stationary quantity, function of the material and the electric field. The other unique feature of the dispersive transport is the universality of its transport characteristics with respect to parameters which do not affect the dispersion of its characteristic times. For example, the time dependent growth of trapped hole concentration (or equivalently flatband voltage shift) due to incident ionizing radiation on gate oxides of various thicknesses will have different time scales, but the same overall shape. All the response curves will overlay on each other if they are plotted in the unit of a suitable transit time. Previous experimental characterizations of holes and H⁺ ion transport in oxides have clearly established that the transport is dispersive in nature.¹² Hence, the use of conventional tools, such as the drift-diffusion equation to simulate carrier transport in oxides is questionable.

Modeling of dispersive transport has been successfully done through the use of continuous time random walk (CTRW).⁴⁻⁵ Scher and Montroll developed the original formulations which treat transport of carriers as a series of hops between the localized sites randomly distributed throughout the sample. The problem was simplified by assuming hopping sites in the form of a periodic lattice. The randomness of the hopping process was semi-phenomenologically modeled by assuming a suitable form for the hopping time distribution function \( \phi(t) \). \( \phi(t) \) gives the probability of a carrier making a hop in time \( dt \) out of a lattice site after time \( t \) of its arrival. Scher and Montroll showed that the form of \( \phi(t) \sim t^{-(1+\alpha)} \), where \( \alpha \) is a fitting parameter which characterizes the microscopic transport process, reproduces the characteristic features of dispersive transport. Once \( \phi(t) \) is assumed, the probability of finding a carrier at a lattice point \( l \) at time \( t \), \( P(l,t) \) can be computed using the random walk of the carrier across the discrete lattice points.⁵ Six Moments of \( P(Z,t) \) can be found by taking appropriate solutions for \( P(l,t) \).⁶

However, the complexity of finding an analytical solution for \( P(l,t) \) with the above form of \( \phi(t) \) has led to the following approaches: an analytical solution for \( P(l,t) \) was derived only for \( \alpha=0.5 \) and in the asymptotic time limit,⁷ a trial function solution was computed through matching of moments,⁶ numerical techniques were used which gave solutions for all time.⁸

One of the limitations of the above approaches is their treatment of the electric field. All the above approaches assume a constant electric field in one dimension. In the present paper, we describe a technique based on the numerical method in⁹ which can treat nonuniform variation of the electric field in one dimension. Trapped oxide charges which are typically created due to incident ionizing radiation or due to hot carrier effects make the electric field in the oxide nonuniform. Hence, the influence of nonuniform electric field on dispersive transport of holes and H⁺ ion could be very important. We have illustrated our technique by simulating the dispersive transport of H⁺ ions through the gate oxide of a MOSFET. Dispersive transport of H⁺ ions is particularly important since it is believed that ionizing radiation creates H⁺ ions in the oxide. H⁺ ions thus created slowly drift towards the SiO₂/Si interface and create interface states.²⁻⁹ Number of interface states created per unit time could be estimated by computing the rate of arrival of H⁺ ions at the SiO₂/Si interface since the dispersive transport of H⁺ ions is believed to be the rate limiting process for the interface state growth.²⁻¹⁰ We understand that the theories behind creation of interface states remain controversial,¹¹,¹² although a series of recent experiments by Saks et al. point...
strongly towards H\(^+\) ion theory\(^{3,0}\). In the present paper we have used H\(^+\) ion transport simulation in the oxide as an example to illustrate the importance of treating nonuniform electric field in dispersive transport rather than investigating the validity of the H\(^+\) ion theory of interface states generation. Besides being useful in simulating device degradation due to ionizing radiation, the dispersive transport approach will be very important to simulate hot carrier degradation of the oxide in a MOSFET.

II. SIMULATION APPROACH

Following\(^4\) the treatment of hopping transport is first simplified by discretizing the sample into a lattice of boxes.\(^5\) Electric field within each box is assumed constant, but could vary between boxes. A carrier hops only between neighboring boxes. The average separation between two neighboring boxes is taken approximately equal to the mean separation between hopping sites in the sample. In our example, it was taken equal to 0.26 nm following\(^12\) which suggests that H\(^+\) ions hop through local bonding between neighboring oxygen atoms. We have used \(\psi(t) = (tW_m)^{-(1+\alpha)}\) as given by Scher et al.,\(^4\) where \(\alpha\) is a measure of the dispersion of the carrier packet and varies between 0 and 1. \(W_m\) is a constant which is related to the rate of transfer of carriers from site to site. We have built in the dependence of hopping on the electric field by treating \(W_m\) as a function of the magnitude of the electric field.

The spatial hopping probability between neighboring boxes is treated in a similar manner as in.\(^5\)\(^8\) We have assumed isotropic nearest neighbor hopping under zero field, i.e., equal probability in each of the six directions. Under the presence of the electric field, the probability of a carrier hopping opposite to the electric field direction was assumed negligible since the hopping probability depends exponentially on the magnitude of the electric field.\(^12\) The above assumption will be acceptable in most cases since the oxide electric field is typically quite high. The probability of a carrier hopping along the directions transverse to the electric field was assumed not affected by the electric field.\(^5\)\(^8\)

With the above scheme, we shall first illustrate our technique in case of a step electric field as shown in the inset of Fig. 1. We begin with the assumption that carriers are injected as an impulse at \(t=0, \epsilon=0\). Afterwards, the same approach is extended to the case of generation of carriers throughout the sample using convolution in space. The probability, \(P(l,t)\) of finding a carrier at any box in the first segment with the electric field \(E_1\) is identical to the case of an isolated segment with uniform field \(E_1\) since the second segment doesn’t affect the transport process in the first segment due to neglect of backward hopping. However, the carriers reaching the boundary of the first segment for the first time (this quantity was called first time transit function, \(F(l,t)\) in\(^4\)\(^5\)\(^8\)) will act as a source for the second segment. Therefore, the probability of finding a carrier at any position \(l\) with the step electric field occurring at \(l_1\) is given by

\[
P(l,t) = G_1(l,t), \quad l < l_1
\]

\[
= \int_0^t F(l_1,t')G_2(l-l_1,t-t')dt', \quad l > l_1
\]

where \(G_1(l,t), G_2(l,t)\) are the Green’s functions for finding the probability of a carrier in segment 1 and segment 2, respectively. Electric fields in segment 1 and 2 are taken into account while computing values of \(G_1\) and \(G_2\). \(F(l,t)\) is the probability of carriers reaching \(l\) for the first time at time \(t\). Equation (1) was solved using Laplace transforms. The expressions for the Laplace transform of \(G(l,t)\) and \(F(l_1,t)\) were found following works of Scher and Montroll.\(^4\)\(^5\) In a similar fashion, we can discretize any arbitrary field profile as a series of step fields and apply the above technique. From \(P(l,t)\) we compute quantities, such as the first moment of the charge distribution or the number of carriers making it to the SiO\(_2\)/Si interface per unit time, etc.

III. SIMULATION RESULTS

As an example to illustrate the effects of nonuniform electric field on dispersive transport, we have simulated transport of H\(^+\) ions through the gate oxide of a MOSFET and computed the normalized interface state growth as a function of time. The proposed technique has two fitting parameters, \(\alpha\) and \(W_m\). \(\alpha\) is a function of the material properties, and needs to be determined once for a given oxide. \(\alpha\) was determined by matching the shape of experimentally observed growth of interface states (\(N_{it}\)) to that of the simulated data.\(^2\)\(^9\) For the present simulation, \(\alpha\) was taken equal to 0.38.

\(W_m\) was evaluated from the published experimental data by observing the dependence of the half growth time (\(t_{1/2}\)) on the electric field. Previous researchers reported \(t_{1/2} \propto L^{1/\sigma_{\alpha}}(\Delta_0 - \beta \sigma_{\alpha})^{-\kappa T}\), where \(L, \Delta_0, \beta,\) and \(\sigma_{\alpha}\) are respectively length of the sample, activation energy for hopping, a constant and electric field.\(^7\) All these parameters are determined from the experimental data provided in.\(^12\) Our simulation shows \(t_{1/2} \propto L^{1/\sigma_{\alpha}}/W_m\). By comparing the above expressions for \(t_{1/2}\), we can derive \(W_m = W_m0e^{-((\Delta_0 - \beta \sigma_{\alpha})\kappa T)}\). Another report\(^10\) suggests power law dependence of the electric field on \(t_{1/2}\) rather than the above exponential dependence. In this

![FIG. 1. Growth of normalized \(N_{it}\) as a function of time under a step electric field (1–6 MV/cm) (circles) and an equivalent uniform electric field (triangles). The initial distribution of H\(^+\) ions were assumed triangular with the peak at the SiO\(_2\)/Si interface.](image-url)
paper, we have used exponential dependence of the electric field on $t^{1/2}$ as reported in\(^2\) although a power law dependence can be incorporated in a similar way.

Once $\alpha$ and $W_m$ are known, $P(I,t)$ was computed which in turn gave us the rate of loss of H$^+$ ions to the SiO$_2$/Si interface. The growth of $N_{it}$ was taken proportional to the rate of loss of H$^+$ ions to the SiO$_2$/Si interface. The validity of our approach was first confirmed by comparing our results under uniform field with different methods of solution described in the introduction. These showed excellent fits.

To demonstrate the effect of nonuniform electric field, we have first simulated growth of $N_{it}$ due to irradiation under a model step electric field in a 20 nm oxide. A step electric field could occur due to presence of a charge sheet in the oxide. Figure 1 compares the growth rate of $N_{it}$ under the step field and the equivalent uniform field. Uniform field was computed assuming the same potential difference across the oxide as in the case of the step field. The initial distribution of H$^+$ ions was assumed triangular with peak at the SiO$_2$/Si interface.\(^3\) This type of H$^+$ ion distribution causes maximum growth of $N_{it}$ and could occur if gate bias is positive during irradiation. Figure 1 shows that the growth of $N_{it}$ in the case of the nonuniform electric field is faster since carriers near the SiO$_2$/Si interface see a much higher electric field. We can generalize the above approach for an arbitrary non-uniform electric field. For example, we have simulated a more realistic case where a Gaussian distribution of trapped charge was assumed near the SiO$_2$/Si interface of a soft oxide. The peak of the of the distribution is located 5 nm from the SiO$_2$/Si interface and the sheet density of the trapped charge is assumed to be $10^{13}$ cm$^{-2}$. Poissons’ equation was solved to get the field variation which is shown in the inset of Fig. 2. Figure 2 shows the effect of nonuniform electric field on the growth rate of $N_{it}$ as compared to an equivalent uniform electric field. Nonuniformity in the electric field strongly affects the growth rate of $N_{it}$ as in the previous example. Our simulations show that the extent of the effect of nonuniform electric field depends on various factors, such as electric field distribution, initial distribution of carriers, etc. In the above example, the CTRW equation was not solved self-consistently along with the Poissons’ equations since the number of H$^+$ ions is generally too small to affect the electrostatics in the oxide.

IV. CONCLUSION

In this paper, we have extended the CTRW based approach of Scher and Montroll to include nonuniform variation of the electric field in one dimension. The inclusion of nonuniform variation of the electric field in the CTRW framework is important since the electric field could be highly nonuniform due to trapped charges in the oxide. In case of two dimensions nonuniformity of the electric field arises not only due to trapped charges but also due to various bias conditions. Future research should be focused on a more generalized approach that treats two-dimensional electric field variation without neglecting backward hopping.

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