CLUSTERS IN IONIZATION TRACKS OF ELECTRONS IN SILICON DIOXIDE

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ABSTRACT

An electron transport code is used to generate electron tracks in silicon dioxide. The location of all ionizing interactions is recorded and the distances between each pair of locations calculated. Application of elementary cluster analysis reveals the clustered nature of such tracks. The results for 600 keV primary electrons show a cluster pattern not compatible with the assumptions of columnar recombination or geminate recombination.

INTRODUCTION

The spatial distributions of holes and electrons left in the wake of an energetic electron play a primary role in the determination of the amount of initial recombination which occurs in silicon dioxide exposed to ionizing radiation. For primary electron energies greater than a few keV, the track consists of a sequence of clusters of holes and electrons and does not represent the averaged continuous column so frequently taken in the literature and which is a primary assumption of Jaffe (1) columnar recombination. The clustered character of tracks in insulators is exhibited here in an example calculation based upon a full Monte Carlo representation of a 600 keV primary electron incident on a 1 micron thick slab of SiO2.

The techniques which are used in the determination of the numerical sizes, νo, and frequencies of occurrence of the clusters are (1) the distance matrix of cluster analysis (2,3) or the proximity function of Kellerer (4). With these one can determine the distribution function, f(νo), which can then be incorporated into the process of averaging over tracks.

The structure of electron tracks has considerable bearing on both geminate and columnar recombination models. Onsager's (5) derivation of the geminate model and the oft quoted work of Pai and Enck (6) both presume a uniform, isotropic distribution of non-interacting pairs. It is shown below that this may become a reasonable assumption for applied fields greater than 10⁶ volts/cm. The exhaustive work of Hughes (7) shows the inability of the geminate model to represent experimental data with a single νo value for all applied field strengths. It is shown below that multiple charge correlation effects on recombination is a probable cause.

Over the years a primary deficiency has been noted with regard to Jaffe columnar recombination: the assumption of uniform continuous linear track density. The errors which stem from this hypothesis were revealed by Lea (8) in 1934 and 1940 comparing ionization chamber results of alpha particles and β particles with the theory. Lea provided a way to patch up columnar recombination by the introduction of spherical clusters as a precursor to the columnar phase. The technique shown below provides a basis for calculation of recombination by determining the probability of cluster sizes.

Generation of Tracks

The electron tracks in this work were generated by the MCSS (Monte Carlo Single Scattering) code provided by S. Woolf of Arcon Corp (9). The boundary conditions were: A primary energy of 600 keV, 1 micron thick SiO2 slab and normal incidence as shown in Fig 1. The cross sections for energy loss and angular scatter were obtained from R. Hamm (10) of ORNL. The locations of all hole sites were recorded as well as the "final" sites of the electrons. The holes were frozen at their creation sites, the electrons were transported to an energy of .25ev. The amount of energy transferred at each ionization site was also recorded. Below ionization threshold (8.9 ev) the electrons were transported using the angular scatter cross section value at 9ev and using CSDA based on the ΔE/Δx loss via optical phonons. Radial distributions with end point energies of lev and .25ev were indistinguishable. Resulting

![Fig 1. Boundary conditions for calculations. Final locations of all electrons and holes are determined. Mean values were ~ 6 primary ionizations and ~ 20 total ionizations per track, mean ΔE/Δx = 3.72 MeV/cm and w (ev/e-h pair) = 18.4 ev.](image-url)

Clusters

The origin of the clusters lies in the compound- ing of the two probabilities in Fig 2. The intervals between primary ionizations are distributed along the axis of the track according to e^-βλ. λ is the total mean free path for primary ionization as shown in Fig 3. The energy transfer in Moeller scattering is governed by a 1/Q² (Q is the energy transferred) factor which leads to mostly low energy secondaries, which in turn have mean free paths for ionization small compared to the primary. In this way, coupled with the increased angular scatter cross section at low energies, tertiary etc ionization sites are constrained to lie close to the primary sites. The first collision energy losses by the 600 keV primary are shown in Fig 4. To exhibit the clustered nature of the tracks one can use a technique from cluster analysis called a similarity or distance matrix. In the distance matrix procedure one calc-
ulates the distance between all holes' (electrons') final sites in the track. The distances are assembled in a square matrix, with rows and columns ordered in the sequence of occurrence along the track (e.g. in order of increasing z axis coordinate).

Moeller Scattering:

\[
\frac{d\sigma}{dQ} = \frac{e^4}{E^2} \left\{ \frac{1}{Q} + \frac{(Q - X)^2}{2 - X^2} \frac{1}{E - Q} \right\}
\]

\(Q = \text{Energy transfer}\)

\(\sigma_{\text{max}} = E/2\)

Primary Collision Site Spacing

\[\Delta S = -\lambda p(e \ln \zeta)\]

\(\lambda = \text{Random number 0-1}\)

Mean free path for ionization

Fig 2. Probabilities which lead to clustering. Expression indicates that \(\lambda p\) is energy dependent.

INVERSE MEAN FREE PATH FOR PRIMARY IONIZATION

\[\sigma_{\text{INEL}} = \rho = \frac{1}{\lambda p}\]

Fig 3. The inverse mean free path for electrons in Si02. Curve peaks at ~ 150 eV. Value increases a factor of 15 between 600 keV and 10 keV. \(\lambda p\) at 600 keV = 2200 Å.

Such a matrix has two properties to reduce the number load. The diagonals are zero (there is zero distance from a hole site to itself) and the matrix is symmetric hence, the lower triangular is ignorable. One obtains an upper triangular matrix of correlation distances as in Fig 5. The actual z axis locations of the sites is shown on the row above the matrix.

In the example shown a total of nineteen (19) holes were created along the track. The intuitive notion about a cluster, that distances between members of a cluster are smaller than distances between non members, is correct. So, to exhibit the clusters, one throws away the large numbers and sets to zero all elements of the matrix greater than some chosen value. In Fig. 6 the results are shown for a distance of 500Å. The letter \(w\) replaces the actual number to permit display of the matrices in less space. The rule of membership in these clusters is that the members are within 500Å of each other. The distances between clusters is not contained in the matrix but the locations are shown in the bottom legend.

Fig 4. Primary energy loss distribution. Region to the right of peak follows \(1/Q^2\) of Moeller cross section.

Fig 5. Distance matrix for distances between holes in single 600 keV primary history. Top row of numbers is Z axis coordinate of hole.
Fig 6. Clustered nature of holes in track. W replaces actual distance value of Fig 5. Columns in which no W appears are isolated by distances greater than 500 Å. Readout shows one central cluster size 11, 2 clusters size 3, 2 isolated holes size 0.

Fig 7. Hole clusters for different history than Fig 6. Loss of correlation with decreasing distance parameter is not great. Cluster centroids on Z axis are shown on bottom legend.

Fig 8. Frequency function, \( f(\nu_0) \), for occurrence of clusters, size \( \nu_0 \).
Fig 9. e-h distance matrix. Multiple correlations at small distances are displayed along the track. The result is a rectangular, non-symmetric matrix of distances of separation. Applying the technique above, zeroing elements greater than the chosen correlation distances, yields the patterns in Fig 9. An important feature of these groupings is the decrease in cluster size with decreasing correlation distance. This correlation feature has an impact on recombination rates as shown in the next section.

Some of the resulting numbers are instructive. With a correlation distance of 20Å only 35% of the holes are found singly, the remaining 65% are found in groups of 2, 3 etc. At 50Å only ~20% are singly located. Thus, in spite of a low LET primary, the clustered deposition causes multiple correlation to be the common condition. This result is in considerable contrast to assumptions in the literature based on the notion of continuous uniform energy deposition. See the discussion in the 1984 paper of Oldham (II) for example on using LET for a basis as to the applicability of the Onsager (giminate) model.

Clusters and Recombination Models

Geminate Recombination as developed by Onsager (5) represents a recombination solution based upon Brownian motion in the presence of the electric fields between point charges and an applied field. A primary assumption of the model is that charges only interact as isolated pairs. That such an assumption does not characterize actual electron track distributions is evident from the above work. Onsager himself was aware of the shortcomings as he wrote in his 1938 paper, "Attractive though this explanation is, I hesitate to accept it as final because the expected variation with the lineal density of ions in the column... refuses to appear."

The effect of clustered pairs vs isolated pairs on the recombination rate is shown in Fig 10. This is work based on a full Monte Carlo time step development performed at the Interuniversity Reactor Institute in the Netherlands (12). The ion pairs were distributed as isolated pairs, doublets and triplets. The increase in the recombination rate due to the several particle aspects is evident and shows the error in treating initial recombination on the basis of summing simple isolated pair results. The results of this difference in recombination rates may not lead to a final difference in the amount of recombination. Only if charge separation increase intrudes in the early time phase, that is one has a sufficiently large external field, will a significant difference in the final result occur. The isolation of charges is dependent on the applied field strength. Point charges in SiO2 separated by a distance of 20Å exert fields of ~105 volts/cm. Thus, in an applied field of the same magnitude, only those charges of approximately this order of separation or less can respond to their coulomb interaction. At
60A the corresponding pair field is \(10^5\) v/cm and at 200A about \(10^6\) v/cm. It is clear from Figs. 7, 9 that as one increases the correlation distance the multiple correlation of the charges increases and from Fig. 10 and ref 12 the recombination rate also increases. The largest distance correlation value related to coulomb effects is given by the Onsager critical length, \(r_c = e^2/4\pi\varepsilon_c\varepsilon_o T\) at which range, \((146A)\), thermal dynamics effects become dominant over coulomb effects. The increase in e-e, h-h and e-h correlation with decreasing applied field will occur independently of track structure details and would be seen in a uniform distribution as well. Modification of geminate recombination to include space distribution effects is not pursued further in this article.

**Columnar Recombination**

The columnar recombination model of Jaffe was modified by Lea (8) to accomodate a cluster precursor phase in the ionization density. The frequency function for clusters in Fig 8 fulfills an important requirement for applications of that theory. The set of assumptions underlying Jaffe theory even when modified by Lea (as averse to uniform distribution along the track) still precludes it from being a viable theory, able to cope with the short ranges and high fields common in microelectronics.

The radial distribution assumption of Jaffe, for instance, is compared to the Monte Carlo result in Fig. 11 and is seen not to be quantitatively correct. It was further pointed out by Kramers (13) that the solution technique of Jaffe was in error at solid/liquid densities and applied fields greater than \(5 \times 10^4\) v/cm. So, while possible, it appears not to be fruitful to pursue the cluster corrected Jaffe recombination model further.

**Summary**

It is shown here that the initial condition assumption of both geminate and columnar recombination models does not conform to actual distributions of electrons and holes for energetic electrons. It is shown how to quantitatively characterize the actual distribution through a cluster probability function. The impact of several e-h pair correlations on recombination is exhibited.

Inclusion of the clustered character of the initial distribution into a physically sound recombination theory is being pursued.

**References**

9. S. Woolf, Arcon Corp.
10. R. Hamm, Health & Safety Research Div., ORNL.

![Fig 11. Radial hole and electron distributions. Curves show number of particles contained in successive cylindrical shells. Differences between Monte Carlo result and Jaffe assumptions are evident. Median radius for electrons is \(40\) A, 75 percentile 70 A. The difference between e and h distributions is due to e transport below ionization threshold.](attachment:image.png)