INFLUENCE OF SURFACE STATES ON THE PERFORMANCE OF THREE-PHASE CHARGE-COUPLED DEVICES

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ABSTRACT

A method, which takes into account the variation of surface state density and capture cross-section with energy, is presented for calculating the transfer loss in three-phase C.C.D.s due to surface state trapping. The results show that surface state loss under the transfer electrodes can be quite significant even when FAT ZEROs are used.

1. INTRODUCTION

Trapping of carriers by interface states makes a significant contribution to transfer inefficiency in all surface channel charge-coupled devices. Attempts have been made to estimate quantitatively the extent of this loss (refs 1,2,3), but in general the simplifying assumptions of both a uniform distribution of surface state density and capture cross-section of the traps have been made in these models. In the analysis that follows a modified method, which takes into account the variation of the surface state density and capture cross-section of the traps in three-phase C.C.D.s, is presented. Calculations for a typical (111) Si-SiO_2 system show that the earlier theoretical models have underestimated the transfer inefficiency, and that in three-phase C.C.D.s, even when FAT ZEROs are employed, the surface state loss under the transfer electrodes can be very significant.

2. THEORY

Though accurate determination of the surface state density and capture cross-section of the traps, which are very near the silicon band edges, has always been a difficult problem, it is fairly certain now that the surface state density increases monotonically as one approaches the band edges and that the capture cross-section of the traps falls very rapidly near the band edges. Though the surface state density appears to increase only by an order of magnitude near the band edge, the capture cross-section is estimated to fall by a few orders of magnitude (ref 4). In order that these variations are taken into account, and also that the exact variation of the occupation level of the traps as a function of energy is calculated at every stage of the transfer cycle, separate equations are initially developed to describe the two processes of filling and emptying of the states. An n-channel device is considered.

For any one particular energy level E (measured from the conduction band) the filling process is given by (ref 1)

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$$\frac{dn_{ss}(t)}{dt} = \sigma v n_s/d\,[N_{SS}' - n_{ss}(t)] \qquad (1)$$

where n_{ss} is the density of filled surface states, N_{SS}' is the density of available states at the energy level considered, n_s is the density of mobile electrons per unit area at the interface in the conduction band, σ is the capture cross-section of the traps corresponding to the particular energy level, v is the average thermal velocity of the carriers and d is the depth of the inversion layer.

$$N_{SS}' = N_{SS}\,[1 + \exp[(E_F - E)/kT]]^{-1} \qquad (2)$$

where N_{SS} is the total density of surface states per unit area per eV at energy E and E_F is the Fermi level corresponding to n_s, i.e.

$$E_F = kT\,\log(N_C d/n_s) \qquad (3)$$

Here N_C is the volume density of the states in the conduction band and kT is the thermal energy in eV.* Equations (1) and (2) specify that after sufficient time has elapsed the trap filling at a given energy will be determined by n_s, i.e. the free electron density. This is in contrast to the assumption, made in the earlier models, that all the states up to the conduction band are completely filled whenever there is a signal charge packet present below the electrodes. Solving equation (1) with the initial condition that at

$$t = 0,\ n_{ss} = f_o N_{SS} \qquad (4)$$

where f_o is the original level of filling of the traps, one obtains the level of filling at E at any time t as

$$f(t) = f_o \exp(-\sigma v n_s t/d) + [1 + \exp[(E_F - E)/kT]]^{-1}[1 - \exp(-\sigma v n_s t/d)] \qquad (5)$$

The emptying process begins as soon as the free charge transfer occurs. Since the quasi-Fermi level falls down to a very low value, the surface states under consideration can potentially all empty. The emptying process is given by (ref 1)

$$\frac{dn_{ss}(t)}{dt} = -n_{ss}(t)\,\sigma v\, N_C \exp(-E/kT) \qquad (6)$$

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*Equation (1) assumes that the value of n_s is not considerably altered by the trapping of carriers. In practice, n_s is of the order of $10^{12}cm^{-2}$ and available trap density is of the order of $10^{10}cm^{-2}$ due to the relatively small change in trap occupancy occurring during the filling and emptying processes: see Fig. 3.

Solving with the initial condition that at t=0, $n_{ss} = f_o N_{SS}$, where f_o now corresponds to the level of filling when the emptying process begins, one gets

$$f(t) = f_o \exp\left[-\sigma v N_C t \exp(-E/kT)\right] \qquad (7)$$

With the help of equations (5) and (7), it is possible to compute f(t) for each energy level in the forbidden band at any one stage of the transfer cycle and to update f(t) for the next time interval to take into account the next stage in the process. Thus after any stage in the transfer cycle, the exact nature of the variation of the level of filling of the states will be obtained. This is in contrast to the abrupt transition in the occupancy level, which is used in the earlier models. Also, whenever a charge packet, either a ONE or a FAT ZERO, is present under the electrodes which are being considered, the filling process is assumed to be the most dominant one and so the emptying process is neglected during these time intervals. f_o is assumed as zero for all levels initially and then is updated using equations (5) and (7) to take into account the stream of FAT ZEROs which run through the device.

In this analysis it is assumed that square pulses are applied to the transfer electrodes and that the free charge transfers instantaneously from one electrode to the next at time intervals of $1/3f_c$ where f_c is the clocking frequency.* For calculating transfer inefficiency by this method, five stages in the transfer process, when a ONE is introduced into a stream of FAT ZEROs, are considered sequentially. The FAT ZERO preceding the ONE is initially assumed to stay under the set of transfer electrodes which are being considered for a time interval equal to $1/3f_c$. With the appropriate values of t, n_s, and f_o the occupation level is determined for each energy level with the help of equation (5). In the next $1/3f_c$ time interval, the FAT ZERO empties and the carriers that are emitted from the surface states will join the FAT ZERO forward due to the asymmetry of the potential distribution under the electrodes in a 3-phase system, (ref 2). f(t) for each energy level is now computed with equation (7), using the values of f(t) obtained at the end of the previous $1/3f_c$ time interval for f_o in these calculations. Again for the next $1/3f_c$ time interval, the FAT ZERO continues to empty and the carriers emitted now will travel backward due to the asymmetric potential distribution as mentioned above to join the following charge packet which is a ONE. Then with suitable values of n_s in equation (5), f(t) is updated when the ONE fills the states and stays for one-third of the total period. The traps empty in the next $1/3f_c$ time interval and the emitted carriers join the ONE forward. The carriers in the next $1/3f_c$ time interval are lost to the ONE. The five stages in the transfer process described above are shown schematically in Fig. 1, where the trap occupancy as a function of time is demonstrated. The charge that is lost by the ONE is determined by the changes in trap occupancy that occur and is given by the sequence

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*In practice, the pulses applied have finite fall and rise times and the rate of charge transfer is dependent on the clocking waveform and the size of the charge packet. Theoretical calculations show that when the size of the charge packet is smaller than the voltage swing can hold, then most of the charge is transferred very early in the transfer period. (ref 5) Therefore the assumption that charge is transferred instantaneously is a valid approximation in the case of fractional charge packets.

$$(4 - 3) - [(2 - 3) + (4 - 5)] = (5 - 2)$$

Hence the number of carriers that are lost by the ONE due to trapping by surface states at any one energy level is determined by the difference in the level of filling after the FAT ZERO emptied in the first $1/3f_c$ time interval and the level of filling after the ONE emptied in its first $1/3f_c$ time interval. Knowing both this difference and the value of surface state density at different energies, the total number of carriers lost and hence the value of transfer inefficiency can be calculated.

3. CALCULATIONS

For one particular case, transfer efficiency as a function of clocking frequency and FAT ZERO size was computed by the above method. The variations of surface state density and capture cross-section with respect to energy for a dry oxide grown on (111) silicon, as reported by Deuling et al. (ref 4) and the equations of Boudry (ref 6) that approximate these particular variations were used in the calculations. They are given in Fig. 2. The charge density of a ONE was taken to be equivalent to 10 volts across a 2000Å thick oxide and the values of v, d and N_C used were 10^7cm sec^{-1}, 100Å and 10^{19}cm^{-3}. The results obtained are given in Figures 3, 4 and 5. Fig. 3 gives the manner in which the level of occupation varies at different time intervals across the forbidden band. The operating frequency in this case is 10^7 Hz and the FAT ZERO is 0.5 times the ONE. Curves F_1 and F_0 indicate the Fermi functions corresponding to the ONE and FAT ZERO respectively and they will give the variation of the filling level of the states if the ONE and FAT ZERO stay under the transfer electrodes for a sufficiently long time. Curve 1 gives the distribution of the occupancy level for a FAT ZERO when it stays for a time interval equal to $1/3f_c$ corresponding to 10^7 Hz. Traps nearer to the conduction band are not filled up to their equilibrium value (F_0); this is due to the rapid decrease in the value of the capture cross-section as one approaches the band edge. Curves 2 and 3 give the variation of the level of filling after the FAT ZERO has emptied in the first and second $1/3f_c$ time intervals. Here again, it is seen that states nearer to the band edge do not empty fully due to their smaller values of σ. Curve 4 illustrates the manner in which the occupation level changes after the arrival of a ONE, and Curve 5 depicts the situation after the ONE has emptied in its first $1/3f_c$ time interval. Farther from the band edge, Curve 5 almost merges with Curve 2 but nearer to the band edge there is a significant difference between the two curves. As stated earlier, with this difference in the level of filling for each energy and by taking the corresponding value of surface state density at that energy, the total transfer loss is calculated. The surface state density increases near the band edges and so at higher frequencies, when the states have less time to empty, the transfer loss is expected to be large. Fig. 4 gives the transfer inefficiency as a function of frequency when the FAT ZERO is 0.5 times the ONE. For comparison the case in which N_{SS} and σ are constant throughout the band is also given (Curve B). Fig. 5 gives the variation of inefficiency with respect to FAT ZERO size when the operating frequency is 10^6 Hz. Curve A is when the variation of N_{SS} and σ are taken into account and Curve B is for the case when N_{SS} and σ are assumed constant. There is clearly a significant difference between the two curves. From Curve A, it is seen that the filling and emptying of the states near the band edge is the major loss mechanism and thus a change in FAT ZERO size does not alter the value of inefficiency significantly.

The effect of the variation of the size of ONE on transfer inefficiency was also studied in this analysis. It was expected that if the size of the ONE charge packet was reduced, the fluctuations in the Fermi level during device operation would take place farther away from the band edge, thus avoiding interaction of the mobile carriers with the traps of low capture cross-section. It was hoped that this would reduce the loss due to trapping. However, the transfer inefficiency is defined as the ratio of trapped charge to signal size, and hence it does not necessarily follow that reducing the trapping by reducing the signal size will decrease the inefficiency. In fact, the calculations showed that for a frequency of 1 MHz and a FAT ZERO ratio of 0.5 reducing the signal size from 10V to 1V improved the inefficiency from 2.6×10^{-3} to only 1.6×10^{-3}.

These results present another interesting physical problem. The use of the normal Shockley-Read-Hall statistics and the experimental values of the capture cross-sections of the surface states produces a situation in which some states close to the conduction band have longer emptying time constants than some states deeper in the band gap. This implies that at the beginning of the emptying process, some of the surface states close to the band edge remain filled when those below them are empty (as shown clearly in Fig. 3). This raises the possibility that these states with rather long emission times to the conduction band could empty by a two-stage process: (1) by losing their electrons to the empty surface states below them and (2) these lower states emptying the electrons subsequently to the conduction band. Two conditions have to be met for this to occur. Firstly, the surface states would have to be close enough together spatially for their electron wave functions to interact, and secondly the sum of the emptying time from the higher to the lower state and the emptying time from the lower state to the conduction band would have to be smaller than the emptying time from the higher state to the conduction band. However, for a surface state density of say $10^{12} cm^{-2} eV^{-1}$, the average distance between the surface states will be of the order of 100Å. As they could only communicate by a 'diagonal' tunnelling process involving phonons (ref 7), any interaction seems unlikely and we feel that the model used in these calculations is a realistic one.

4. CONCLUSION

It is clear from these results that if accurate predictions of charge transfer inefficiency are to be made, the values of surface state density and capture cross-section as a function of energy must be well established. The values of N_{SS} and σ used in the present calculations are probably the most reliable data yet available for the $Si\text{-}SiO_2$ system using dry oxidation of (111) orientation silicon and, by using this data, it can be seen that, for 3-phase C.C.D.s, the charge loss under the transfer electrodes due to surface state trapping cannot be neglected. This is mainly due to the very small capture cross-section of the traps near the band edges, and their consequent slow rate of emptying; this was not taken into account in the previous models and thus led to their underestimating the loss due to trapping. As yet there is little experimental information available with which to compare the above theory because the most detailed experimental results of Kosonocky and Carnes (ref 8) are for 2-phase devices. However, the results of Tompsett (ref 2) on 3-phase devices using (100) substrates, and consequently having low surface state densities indicate that the introduction of a 50 per cent. FAT ZERO only reduces the inefficiency by a factor of about 2 rather than by two orders of magnitude as predicted by assuming uniform N_{SS} and σ; see Figure 5.

In addition to the trapping under the transfer electrodes discussed above, as pointed out by Tompsett (ref 2), there will be regions at the edges of these electrodes and in the inter-electrode gaps where surface state trapping effects are likely to be even larger. Thus in surface channel C.C.D.s surface state trapping is expected to be a major contribution to charge transfer inefficiency.

Attempts are now being made to test the above theoretical predictions by measuring the transfer efficiency as a function of surface state density in 3-phase aluminium gate C.C.D.s. In these devices the surface state densities are being varied by the use of low temperature hydrogen/nitrogen annealing treatments, and by the use of (111) and (100) silicon substrates. The density and distribution of the states are being obtained by quasi-static capacitance measurements of an on-chip M.O.S. capacitor, and it is hoped that some of these results will be available at the time of the conference.

5. ACKNOWLEDGEMENT

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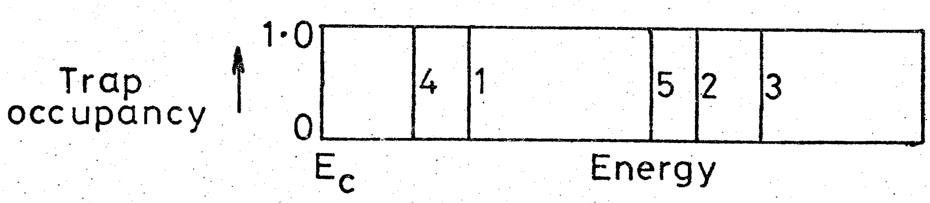

Figure 1.

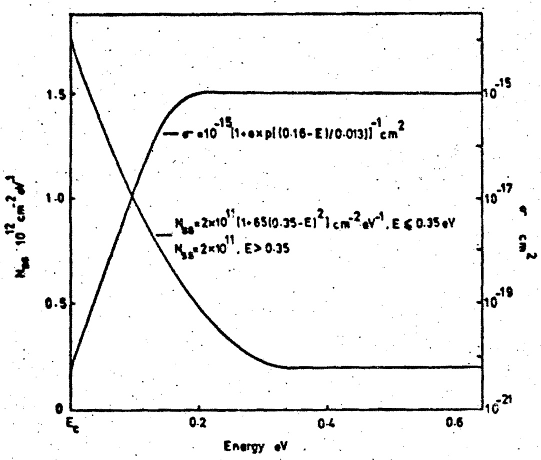

Figure 2

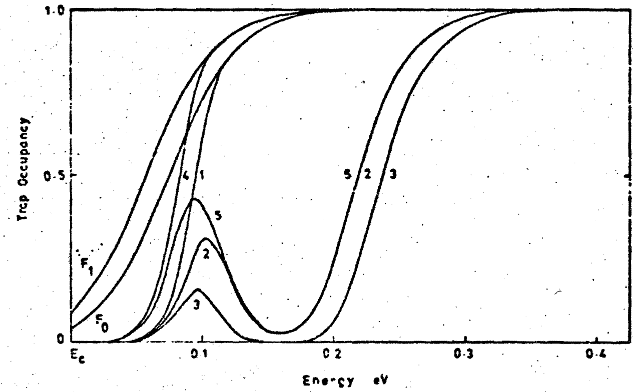

Figure 3

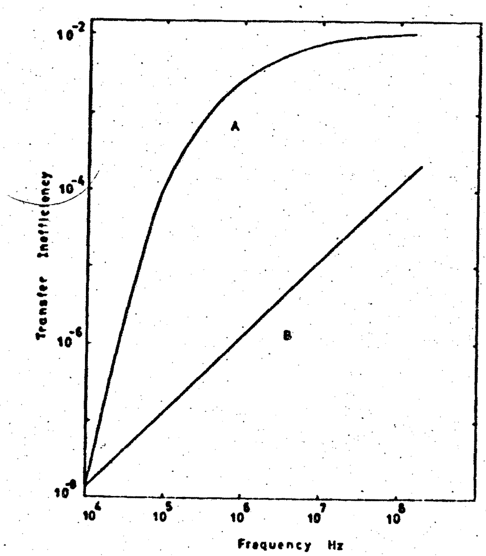

Figure 4

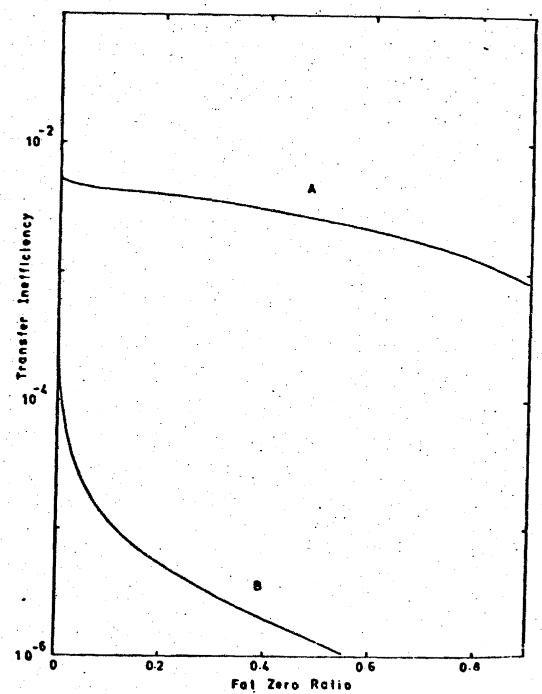

Figure 5

FIGURE CAPTIONS

Figure 1: Schematic representation of the change in trap occupancy

1 - FAT ZERO filling the traps for $1/3f_c$ time interval

2 - FAT ZERO emptying in the next $1/3f_c$ time interval. These carriers join the FAT ZERO forward.

3 - FAT ZERO emptying for a further $1/3f_c$ time interval. These carriers join the ONE backwards.

4 - ONE filling the traps for $1/3f_c$ time interval.

5 - ONE emptying in the next $1/3f_c$ time interval. These carriers join the ONE forward.

Figure 2: Plots of N_{SS} and σ versus energy, as used in the calculations. the equations describing these plots are:

$$N_{SS} = 2 \times 10^{11} \left[1 + 65(0.35 - E)^2\right] \text{cm}^{-2}\text{eV}^{-1},\ E \leq 0.35 \text{ eV}.$$

$$N_{SS} = 2 \times 10^{11} \text{ cm}^{-2}\text{eV}^{-1},\ E > 0.35 \text{ eV}.$$

$$\sigma = 10^{-15} \left[1 + \exp[(0.16 - E)/0.013]\right]^{-1} \text{cm}^{-2}.$$

Figure 3: Trap occupancy at different stages of clocking. f_c is 10^7 Hz, ONE charge packet is equivalent to 10 volts across 2000Å oxide and FAT ZERO ratio is 0.5. F_1 and F_0 give the equilibrium Fermi distributions for the ONE and the FAT ZERO respectively.

1 - FAT ZERO filling the traps for $1/3f_c$ time interval.

2 - FAT ZERO emptying in the next $1/3f_c$ time interval.

3 - FAT ZERO emptying for a further $1/3f_c$ time interval.

4 - ONE filling the traps for $1/3f_c$ time interval.

5 - ONE emptying in the next $1/3f_c$ time interval.

Figure 4: Transfer inefficiency as a function of clocking frequency (with FAT ZERO ratio being 0.5)

A - N_{SS} and σ distributions as shown in Fig. 2.

B - N_{SS} and σ distributions assumed to be uniform across the silicon energy band gap.

Figure 5: Transfer inefficiency as a function of FAT ZERO ratio ($f_c = 10^6$ Hz)

A - N_{SS} and σ distributions as shown in Fig. 2.

B - N_{SS} and σ distributions assumed to be uniform across the silicon energy band gap.