# The Effects of a Multiple Carrier Model of Interface Trap Generation on Lifetime Extraction for MOSFETs

W. McMahon, K. Matsuda[1], J. Lee, K. Hess, J. Lyding

Beckman Institute, University of Illinois at Urbana-Champaign
Urbana, IL 61801, USA, wjmcmahn@uiuc.edu

## ABSTRACT

An isotope effect in the slope of the substrate current versus lifetime requires a model beyond the standard single carrier lucky electron model typically used for MOSFET lifetime extrapolation. A multiple scattering model is developed which allows us to explain this effect. A nonlinearity in the drain current vs. device lifetime curve similar to the one predicted by our model has already been observed by the IBM group.

***Keywords***: interface state generation, lifetime extrapolation, deuterium

## 1 INTRODUCTION

The substrate current has frequently been used as an extrapolation tool for hot carrier interface state generation (HCI) in n-channel MOSFETs [1]. There is an intimate relation between the substrate current and the distribution of high energy carriers, because the substrate current represents the number of impact ionized (II) holes that have been generated at the drain end of the channel [2], and thus it faithfully represents the number of "hot" electrons, where "hot" in this case is defined as the number of electrons with sufficient energy to induce an impact ionization event. In addition, HCI and II are both presumed to involve a single, high energy electron to produce the interface trap or the impact ionized electron-hole pair.

Although there are these similarities between II and the generation of interface traps, the two processes are not the same. The limitations of using a measure of the impact ionization events to estimate the number of interface state generation events must therefore be recognized. In this paper, we discuss the assumptions implicit in the lucky electron model (LEM) of Hu [3] in section 2, and indicate how the LEM applies when deuterium is used instead of hydrogen. In section 3 we indicate the possibility of multiple-scattering events having an effect on lifetime extrapolation for smaller devices, and develop a model which indicates exactly how the substrate current will vary in a multiple-scattering regime. We discuss nonlinearities in the drain current vs. device lifetime curve predicted by this model similar to those observed by Rauch et al. of the IBM group. [4], [5].

## 2 THE LUCKY ELECTRON MODEL AND THE ISOTOPE EFFECT

When attempting to extrapolate the lifetime of MOSFETs from a particular process, the devices are typically stressed at a range of voltages higher than the operating voltage and the lifetimes of the stressed devices are plotted vs. the substrate current [1], [3]. The variation with substrate current is presumed linear and extrapolated down to the desired lifetime. Figure 1 shows two typical experimental data sets of substrate current vs. lifetime for $0.35\mu m$ devices under stress conditions: one set of devices has had the interface states passivated with hydrogen, the other set has had the interface states passivated with deuterium. It is clear from the figure that the slope of the deuterium curve is steeper than the hydrogen curve.

In order to understand whether this difference in slope should be expected from the LEM, we need to go through the derivation of the model in more detail. Similar to the LEM, the substrate current is given by:

$$I_{sub} = C_0 \int_{E_{thresh}}^{\infty} f(E)(E - E_{thresh})^p D(E) dE \quad (1)$$

$$\propto e^{\frac{-E_{thresh}}{kT_e}} \quad (2)$$

where $C_0$ is some constant, $E_{thresh}$ is the threshold energy to II, $D(E)$ is the density of states, $f(E)$ is the electron distribution function, and $(E - E_{thresh})^p$ is a Keldysh-like II cross-section [6].

The manner in which the lifetime of the silicon-hydrogen bonds varies with electron temperature and the threshold energy of the bonds is more difficult to estimate, because the shape of the hydrogen dissociation cross-section is unknown. We can make several assumptions about the type of process involved from experiments done on the desorption of hydrogen by a scanning tunneling microscope (STM) from the silicon (100) interface [7]. We know that a single electron could not give all of its energy to the silicon-hydrogen bond in a direct scattering event because of the large mass differences betweeen the two. Thus, the scattering that results in a desorption event is most likely an electronic

---

[1] Currently on leave from Naruto University of Education 748 Nakashima, Naruto, Tokushima 772-8502, Japan

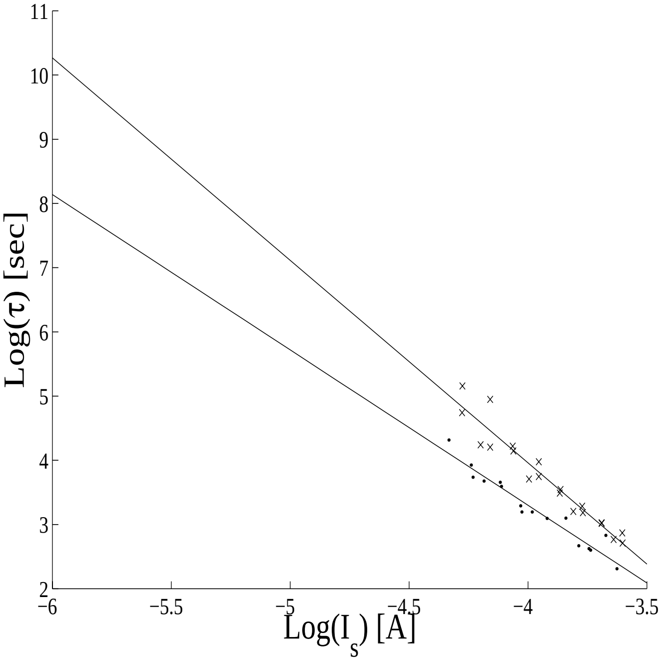

Figure 1: Device lifetime extrapolations for hydrogen and deuterium annealed devices

excitation. This electronic excitation is then followed by the bond evolving along the potential energy surface of the excited electronic state with some probability of desorption before the electron relaxes to the lower energy state. The expression for the rate obtained from Fermi's Golden Rule for such an electronic excitation is very similar to that for II. The only difference is that the valence electron remains localized both before and after the scattering event. From this we might similarly expect a Keldysh-like cross-section for this electronic excitation. The rate of desorption is determined by multiplying this electronic excitation rate by the probability that the bond breaks once it is excited and then integrating the product over the incoming electron energy. The best guess that we can get for the shape of the total function for the rate of bond desorption versus electron energy is from the STM data, from which we know that the total desorption cross section is roughly an exponential function of electron energy [8]. Thus the lifetime for either a silicon-deuterium or a silicon-hydrogen bond is

$$\tau^{-1} = B\int_{E_b}^{\infty} e^{CE} f(E)D(E)\,dE \tag{3}$$

$$\propto e^{(C-1/kT_e)E_b} \tag{4}$$

where now $E_b$ is the threshold for the creation of an interface trap (presumably related to the silicon-hydrogen bond energy). $B$ and $C$ are constants. $C$ is probably different for deuterium than for hydrogen. This lifetime can now be expressed in terms of the substrate current as

$$\tau^{-1} \propto e^{CE_b} I_s^m \tag{5}$$

where $m$ is the ratio of the barrier height for interface trap creation to the threshold for impact ionization. The slope of either curve in Figure 1 should therefore represent the ratio of $E_b$ to $E_i$. But isotopes have exactly the same potential energy surfaces, and it is the potential energy surface which defines the barrier height. The question remains, then, why the slope for deuterium should be different from the slope for hydrogen. We resolve this question in the following section with a multiple scattering model.

## 3 MULTIPLE-CARRIER MODEL

As device sizes diminish, the channel depth also diminishes, but the current density through that channel depth may stay the same or even increase. This implies an increasing number of electrons interacting with the silicon-hydrogen bonds at the interface, and could potentially have effects on the reliability of the device. It is known from the aforementioned STM experiments that the number of bonds broken per electron increases with increasing current at electron energies lower than the expected threshold energy for desorption. That is to say, the lifetime of those bonds is a nonlinear function of the current for sufficiently high currents and low energies. Considering that the mechanism for hot carrier interface state generation is essentially the same, i.e. electrons breaking silicon-hydrogen bonds at an interface, it is clear that at sufficiently high currents, the lifetime of silicon-hydrogen bonds at the interface will similarly be nonlinear in the current. The STM results have been modeled in a low energy, high current regime, and in a high energy, low current regime [7], but if devices begin to see a nonlinear effect with current, they will be in an intermediate regime. It is this regime that we wish to model with our multiple electron model.

### 3.1 Rate Equation for Bond Breaking

The dispersal of the silicon-hydrogen bonds at the interface is wide enough such that each bond dissociation should be independent of the other bonds. As such, we expect the rate equation for bond dissociation to be first order in the number of silicon-hydrogen bonds.

The lifetime for any given device is typically on the order of 10 years, and the total number of dangling bonds required for device failure is very small, thus we expect each bond to have a relatively long lifetime. In comparison, the lifetime for a single phonon mode is on the order of $10^{-8}s$. The huge disparity between the lifetime of a bond and of a phonon mode implies that the ensemble of bonds will reach a steady state distribution of phonon excitations very quickly in comparison to the time taken for a bond to dissociate. We make the assumption that there are independent probabilities for the bond to dissociate from any given phonon mode. Finally, we expect the dissociation event to take place due to a rare electronic transition induced by a single electron. Under these conditions, we can write the rate equation for bond dissociation as:

$$\frac{dN}{dt} = N\sum_{i=0}^{N_p}\tau_i^{-1} = N\sum_{i=0}^{N_p}[P_i R_{ei}] \tag{6}$$

Where $N$ is the number of silicon-hydrogen bonds, $P_i$ is the steady state probability of occupation of the $i$th vibrational state of the bond. $R_{ei}$ is the probability of an electronic excitation followed by desorption from the $i$th vibrational excited state. If we assume a truncated harmonic oscillator model for the phonon levels (similar to [7]), $N_p$ is the total number of phonon leveles. If we additionally assume that the only phonon levels that enhance $P_e$ are the stretching modes of the bond, and we use a barrier height of $3.0eV$, then $N_p = 3.0eV/0.25eV = 12$.

## 3.2 Steady State Vibrational Distribution

We need the current dependence of $P_i$, the probability of being in a particular vibrational state in the steady state. This is essentially the same problem as the STM excitation of a silicon-hydrogen bond [9]. First we assume that no dissociations happen through vibrational transitions to the $N_p + 1$ level. If this is the case, then we are left with a hierarchy of rate equations:

$$\frac{dn_i}{dt} = P_d n_1 - P_u n_0 \tag{7}$$

$$\frac{dn_i}{dt} = P_d(n_{i+1} - n_i) - P_u(n_i - n_{i-1}) \tag{8}$$

where $P_d$ is the probability of a vibrational level getting de-excited from the $i$+1 level to the ith level, $P_u$ is the probability of a vibrational level getting excited from the ith level to the $i$+1 level. We assume that the transition probability above the $N_p$th level is sufficiently small such that an infinite hierarchy of such equations is appropriate. If this is the case, then at steady state we can see that

$$\frac{n_i}{n_0} = \left[\frac{P_u}{P_d}\right]^i \tag{9}$$

There are two pieces to each of $P_u$ and $P_d$, the part which is dependent purely on excitation and decay of phonon modes induced by the lattice, and a piece purely for the stimulation and emission of vibrational modes by incoming electrons. We can get the lattice-induced part by considering the system in equilibrium. For a system in equilibrium, $P_u$ and $P_d$ will just be $exp(\frac{\hbar\omega}{kT})/\tau_p$ and $\tau_p^{-1}$ respectively, where $\tau_p$ is the phonon lifetime.

We must add the probabilities for excitation and de-excitation by incoming electrons to the lattice part, so that we get

$$P_u = \int j_d\sigma_v dE_e + \frac{exp(\frac{\hbar\omega}{kT})}{\tau_p} \tag{10}$$

$$P_d = \int j_d\sigma_v dE_e + \frac{1}{\tau_p} \tag{11}$$

where $\int j_d\sigma_v dE_e$ is the integral of the electron current density ($j_d$) with the cross-section ($\sigma_v$) of excitation of a phonon mode integrated over all electron energies. The rate for de-excitation is assumed to be the same. We assume that this rate will be proportional to the drain current and henceforth write it as $I_d f_v$ where $f_v$ is the fraction of electrons induceing an excitation

$P_i$ in equation 6 is then just

$$P_i = \left[\frac{P_u}{P_d}\right]^i = \left[\frac{I_d f_v + \frac{exp(\frac{\hbar\omega}{kT})}{\tau_p}}{I_d f_v + \frac{1}{\tau_p}}\right] \tag{12}$$

## 3.3 Probability of Electronic Excitation/Bond Dissociation

We next need to estimate $R_{ei}$, the rate of dissociation from a particular phonon level. We again assume that some fraction of carriers will induce desorption, but that there will be an enhancement of that fraction for each phonon level. We assume that this enhancement is exponential based on the yield of hydrogen as a function of electron energy for the STM induced desorption of hydrogen from the silicon (100) surface [8]. Using this, we get

$$R_{ei} = A^i I_d f_d \tag{13}$$

And the rate of silicon-hydrogen bond breakage is

$$\tau^{-1} = \sum_{i=0}^{N_p}\left[\frac{I_d f_v + \frac{exp(\frac{\hbar\omega}{kT})}{\tau_p}}{I_d f_v + \frac{1}{\tau_p}}\right]^i A^i I_d f_d \tag{14}$$

Using this model, we can explicitly see where the lifetime becomes a nonlinear function of the current, and how this transition is considerably later for deuterium than for hydrogen, as seen in Figure 2. Bending similar to this has been seen by the IBM group [5]. We call the region where bending begins the "multiple phonon" (MP) regime.

## 3.4 Effects of Multiple Carrier Model on Slope

By expressing our model in terms of the substrate current rather than the drain current, we can now examine how the slope of substrate current vs. lifetime

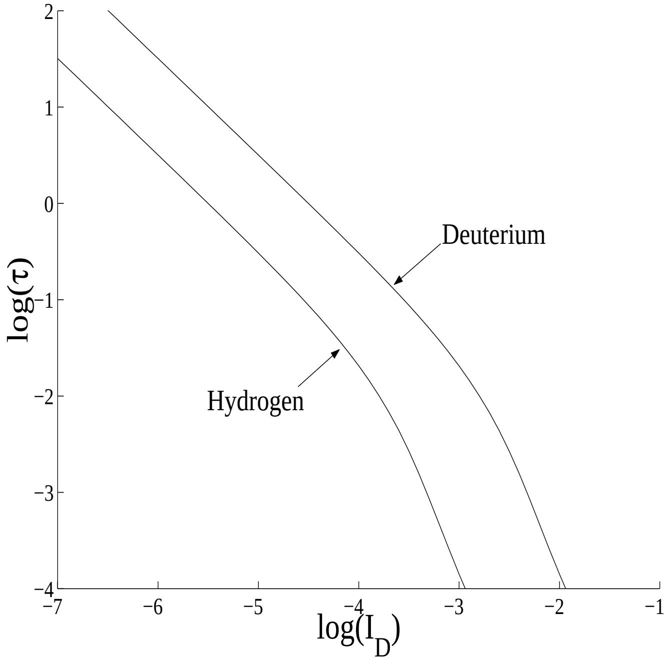

Figure 2: Projected lifetime vs. drain current within a multiple carrier model.

will vary in the MP regime, and why the slope is lower for hydrogen than for deuterium. The onset of the MP regime occurs when

$$\tau_p^{-1} > I_d f_v > exp(\hbar\omega/kT) \quad (15)$$

For this level of drain current, $P_1$ will be considerably larger than all of the other $P_i$'s, and so the lifetime looks like:

$$\tau^{-1} \approx I_d f_d + A I_d f_d I_d f_v \tau_p \quad (16)$$

But $I_d f_d$ in the first term will be proportional to $I_s^m$ where m is $E_b/E_i$ as expected from the LEM. $A I_d f_d$ in the second term, however, will be proportional to $I_s^{\frac{E_b-\hbar\omega}{E_i}}$. Within a two temperature model, the integral for the excitation of a phonon mode (or $I_d f_v$ in our model) could similarly (but more approximately) be written in terms of the substrate current, and will be proportional to $I_s^{\frac{\hbar\omega T_2}{E_i T_1}}$ where $T_1$ and $T_2$ are the electron temperatures at the low end and the high end of the electron energy distribution, and $T_2 >> T_1$. Hence the exponent of $I_s$ in the second term will be lower than the first by $\hbar\omega/E_i$. The farther into the MP regime the device is stressed, the lower the value of $m$.

## 4 DISCUSSION

Recently, a model by the IBM group [4] has also considered the possibility of changes in the slope of the lifetime vs. substrate current curve. Their model also causes a reduction in $m$ from multiple electron-electron scattering events, but deals with electrons gaining energy from scattering off of other high energy electrons in the channel. The primary distinction between our model and theirs is that ours will result in an isotope effect in $m$, whereas one would not expect to see such an effect in theirs. The onset of the electron-electron scattering effect is defined by the applied source-drain voltage (when it is below the threshold for interface trap generation but above the threshold for impact ionization), whereas the onset of the MP effect is defined by the current. It is entirely conceivable that both of these nonlinearities in $m$ will occur in the low voltage, high current regime.

The MP model presented above depends intimately on parameters which have to do with the dynamics of the silicon-hydrogen or silicon-deuterium bond. It is known that the deuterium stretching mode has a shorter lifetime than hydrogen stretching mode, and thus we expect that the steady state occupation of higher modes for deuterium will be less than for hydrogen. Thus we can expect an increase in the isotope effect for multiphonon regimes. Linear extrapolation of the lifetimes of both hydrogen and deuterium will result in an overestimation of the isotope effect because hydrogen will enter a multiple scattering regime before deuterium, and thus $m$ for hydrogen will increase for lower values of the substrate current, while $m$ for deuterium will remain the same or increase less.

## REFERENCES

[1] E. Takeda, C. Y. Yang, A. Miura-Hamada, "Hot-Carrier Effects in MOS Devices", Academic Press, pp. 79-87, 1995.

[2] S. Sze, "Physics of Semiconductor Devices", John Wiley & Sons, p. 480, 1981.

[3] C. Hu, S. C. Tam, F.-C. Hsu, P.-K. Ko, T.-Y. Chan, K. W. Terrill, IEEE Trans. Elect. Devs. 30, p. 375, 1985.

[4] S. Rauch III, F. J. Guarin, G. LaRosa, IEEE Elect. Dev. Letters, 19, 463, 1998.

[5] S. Rauch III, G. LaRosa, F. J. Guarin, IEEE International Reliability Physics Symposium Proceedings, p. 399, 2001.

[6] J. Bude, K. Hess, J. Appl. Phys. 72 (8), p. 3554, 1992.

[7] Ph. Avouris, R. E. Walkup, A. R. Rossi, R.-C. Shen, G. C. Abeln, J. R. Tucker, J. W. Lyding, Chem. Phys. Letters, 257, pp. 148-154, 1996

[8] T.-C. Shen, C. Wang, G. C. Abeln, J. R. Tucker, J. W. Lyding. Ph. Avouris, R. E. Walkup, Science, 268, p. 1590, 1995.

[9] R. E. Walkup, D. M. Newns, Ph. Avouris, Atomic and Nanometer-Scale Modification of Materials: Fundamentals and Applications, pp. 97-109, 1993.