AIP Applied Physics Letters

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Citation: Applied Physics Letters **106**, 163503 (2015); doi: 10.1063/1.4919100
View online: http://dx.doi.org/10.1063/1.4919100
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# Interface-state capture cross section—Why does it vary so much?

J. T. Ryan, A. Matsuda, J. P. Campbell, and K. P. Cheung[a]
*Semiconductor and Dimensional Metrology Division, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, Maryland 20899, USA*

(Received 8 December 2014; accepted 12 April 2015; published online 21 April 2015)

A capture cross section value is often assigned to Si–$SiO_2$ interface defects. Using a kinetic variation of the charge pumping technique and transition state theory, we show that the value of capture cross section is extremely sensitive to the measurement approach and does not provide any meaningful insight into the physics involved. We argue that capture cross section is neither a physical property of interface defects nor is there any need to assign capture cross section values.
[http://dx.doi.org/10.1063/1.4919100]

The metal–oxide–semiconductor field-effect-transistor (MOSFET) has made possible the incredible growth and ubiquity of microelectronics-based technology. This is, in a very large part, due to the extremely high quality of the Si–$SiO_2$ interface. Conversely, imperfections at the Si–$SiO_2$ interface play important roles in determining overall device performance and reliability. Countless studies have been performed in an attempt to understand their charge capture and emission behavior. The so-called capture cross section, sold as an indicator for interface defect capture efficiency, has been investigated by a large number of techniques with reported values spanning a shockingly wide range ($10^{-12}$ cm$^2$ to $10^{-23}$ cm$^2$, see Figure 1).[1–10] Considering that capture cross section is often viewed as an inherent property of interface states, this alarmingly large range in value clearly requires further investigation.

The problem is multifaceted. The survey of Figure 1 is composed of a variety of measurement techniques, each with their own accuracy limitations and specific measurement conditions. Furthermore, in most samples, the presence of "near-interface" or "border trap" defect states, which can also readily capture and emit charge carriers, pose a great difficulty in measurement analysis. To get a clearer picture, we recently applied a variable duty cycle charge pumping (VDC-CP) methodology to probe the charge capture kinetics directly (as opposed to steady-state techniques like that of spectroscopic charge pumping[12]) and applied it to a sample that is free of "near-interface" defects.[11] This "clean" combination allowed for a detailed investigation of charge capture purely by interface states.[11]

The VDC-CP method measures electron (or hole) capture time constants, $\tau$, as a function of available carrier concentration. For charge-capture studies in the literature,[1–6,8–10] the common practice is to extract a capture cross section value ($\sigma$) from $\tau$ using the following equation:

$$\sigma = 1/(\tau v n), \quad (1)$$

where $v$ is electron thermal velocity and $n$ is carrier volume density. Equation (1) originates from the hard-sphere collision model [the hard-sphere collision model is covered by virtually all chemistry text books. The original reference is not traceable], in which one of the two particle types involved is much smaller than the other. Thus, electrons have been implicitly assumed to be small compared to the size of the defect. Considering the de Broglie wavelength for an electron with thermal energy in silicon is ~10 nm, the model is clearly inappropriate. Additionally, although $v$ is often taken as $10^7$ cm/s, the physical meaning of such a "velocity" in terms of the charge capture process is unclear.

Here, we explain why a transition state theory analysis more appropriately describes the interface state capture process and how it can explain the wildly varied capture cross sections reported in the literature. First, the "reaction" (charge-capture process) must be clarified. Fig. 2 shows the common band diagram picture of an electron in the conduction band (labeled A) being captured by an interface state (labeled B). This picture leads to the common but incorrect conclusion that the electron ends up at B and therefore B is the final state. This cannot be true because charge capture dictates some structural rearrangement and it is physically impossible for the trap energy level to remain unchanged upon capturing an electron. The actual final state is not shown and its energy level has not been investigated.

Both A and B are initial states. Proper description of the process, in the language of transition state theory, is that the empty defect state B absorbs a phonon with enough energy to allow it to form an activated complex with the electron. This activated complex can either fall apart or form a new defect state with the captured electron. Thus, the "reaction" is: *Trap* → *Trap** → *Trap(e)*. The first step is the "activation" step that involves the absorption of a phonon as well as the formation of an activated complex (*Trap**) with an electron. Conservation of energy dictates that the absorbed phonon must have an energy that matches the energy difference between the electron in the conduction band and the initial defect energy state. The second step is to form the final trap state with a captured electron, *Trap(e)*.

The second step of forming the charged defect from the activated complex is fast. Consequently, the kinetics of the reaction are almost entirely controlled by the activation step. We therefore have the rate of change of filled traps ($N_{Fi}$) proportional to the available empty traps ($N_{Ei}$) and the available carriers ($N_C$), i.e.,

$$\frac{dN_{Fi}}{dt} = -\frac{dN_{Ei}}{dt} = c_i N_{Ei} N_C, \quad (2)$$

[a]Electronic mail: kin.cheung@nist.gov

0003-6951/2015/106(16)/163503/3/$30.00 

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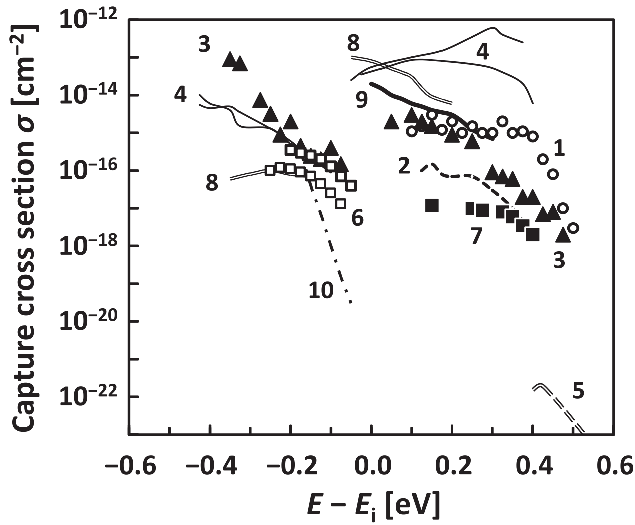


FIG. 1. Reported capture cross section of "interface states" in Si–$SiO_2$ system varies wildly, covering 11 orders of magnitude. Many groups report capture cross section as a function of energy. Labels indicate reference numbers.[1–10]

where $c_i$ is the trap activation rate. In the VDC-CP experiment,[11] $N_C$ is kept constant and the problem becomes pseudo first order in nature with the solution as

$$N_{Fi}(t) = N_{Ei}(0)(1 - \exp(-c_i N_C t)) = N_{Ei}(0)\left(1 - \exp\left(\frac{-t}{\tau_i}\right)\right), \quad (3)$$

where $N_{Ei}(0)$ is the initial concentration of empty traps at energy $E_i$, and

$$\tau_i = \frac{1}{c_i N_C}. \quad (4)$$

Since (2) is a second order reaction, $c_i$ has units of $[\mathrm{M}^{-1}\,\mathrm{s}^{-1}]$, where M is concentration. On the other hand, in the VDC-CP experiment, where the number of defects does not change the kinetics, we can simply treat the problem for a single defect. According to the Eyring–Polanyi equation[13]

$$c_i = \frac{k_B T}{h}\exp\left(\frac{-\Delta E_i}{k_B T}\right), \quad (5)$$

where $k_B$ is the Boltzmann's constant, $h$ is the Plank's constant, and $T$ is the temperature. Equation (5) differs from the Arrhenius's equation by the pre-exponential factor (by a factor of ~2 for silicon), but the effect on the extracted defect energy level is negligible. Combining (4) and (5), we get

$$\frac{1}{\tau_i} = N_C \frac{k_B T}{h}\exp\left(\frac{-\Delta E_i}{k_B T}\right), \quad (6)$$

which allows us to extract the defect energy levels directly from measured time constants. Note that this approach does not require any assumptions or adjustable parameters and, perhaps most importantly, the use of a capture cross section has been completely avoided.

In the recent VDC-CP work[11] and since the defect energy levels have been independently and directly measured using a related steady state spectroscopic charge pumping technique,[12] the transition state theory approach to extracting defect energy distributions has been directly verified. In both the VDC-CP and spectroscopic charge pumping measurements, two peaks indicative of an amphoteric defect were observed with approximately the same peak energy locations and peak breadth. Since the spectroscopic charge pumping technique was performed with much finer resolution, we argued that the agreement is quite good.[11] The important thing to note is that using transition state theory to extract defect energy levels from capture time constant uses no adjustable parameters. Thus, the remarkable correlation is a strong statement of support.

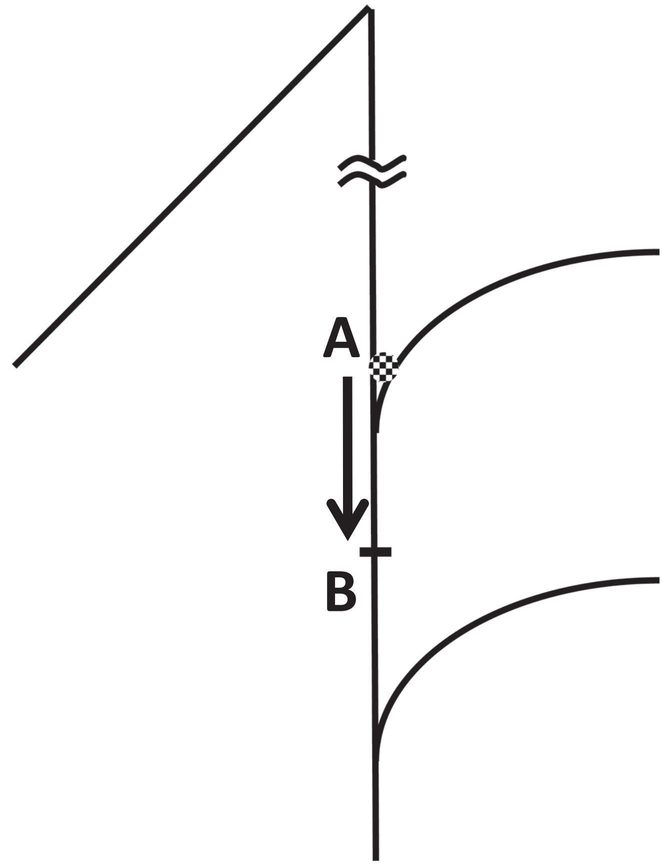


FIG. 2. Schematic illustration of the common band diagram picture of an electron in the conduction band (labeled A) being captured by an interface state (labeled B). Both A and B are initial states with the final state (trap with a captured electron) not shown.

With the capture time constants directly related to the energy change involved in the capture process, we can now explain why the reported capture cross sections values vary so wildly amongst different techniques and measurement methods. Figure 3 shows apparent capture cross section (extracted from Eq. (1)) as a function of the corresponding transition state theory $\Delta E$. The capture cross section value can range from 0.1 $\mathrm{cm}^2$ to $10^{-24}$ $\mathrm{cm}^2$ and is extremely sensitive to the variation in $\Delta E$. This means that the "measured" capture cross section is heavily dependent on how it is measured. Different measurement techniques have different energy windows defined by the particular measurement approach and the specific conditions used.

For example, indicated in Figure 3 are two values of charge pumping inversion half cycle voltage (the

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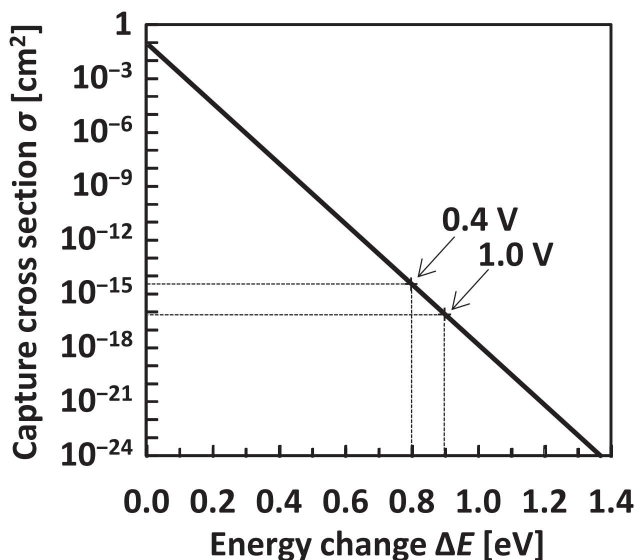


FIG. 3. Capture cross section as a function of energy change ($\Delta E$) involved in the capture process by using Eqs. (1) and (6). $\Delta E$ extends beyond the band gap (1.1 eV) to account for the first sub-band level due to quantum confinement. The indicated charge pumping inversion voltages ($V_{inv} = 0.4$ V and $V_{inv} = 1.0$ V) from our other works[11] are indicated to demonstrate how the capture cross section value can vary significantly, even for voltages above threshold.

accumulation half cycle voltage is constant). While both voltages are above threshold and the difference in $\Delta E$ is relatively small (about 0.1 eV), the capture cross section value varies by almost two orders of magnitude. Additionally, due to quantum confinement, the first sub-band can be located as much as 0.23 eV above the conduction band edge.[14,15] Therefore, an electron getting trapped at a defect state 0.4 eV above the valence band edge can experience a $\Delta E$ ranging anywhere from 0.7 eV to 0.93 eV, depending on the band bending. Based on Eqs. (1) and (6), this translates to as much as four orders of magnitude change in the apparent capture cross section despite the fact that the only difference is the gate voltage. (Similar arguments can be made for cross section extracted from emission experiments. Other than changing available carriers for capture to available empty states for emission, the argument is the same.) This example is within a single set of experiments; when trap states are measured by a variety of measurement methods, the transition state theory $\Delta E$ range is larger and so is the range of hard sphere cross sections. Referring to Figure 1, the various types of measurement techniques (charge pumping, capacitance-voltage, deep level transient spectroscopy, etc.) used and their specific experimental conditions led to the reports of widely different values. As mentioned earlier, the different accuracy limitations of the measurements and the possible presence of bulk and/or border traps contribute as well.

The above discussion suggests that the customary use of capture cross section to characterize an interface defect is meaningless. Not only is the hard-sphere model inappropriate for the problem at hand but also it provides no meaningful insight and the extracted value is nowhere near being a unique parameter. In too many situations, capture cross section is used as a fudge factor to gloss over inconsistent results or models.

Our kinetic treatment suggests that, at least for charge capture by interface defects, once the defect energy is known, all the kinetics can be explained without invoking a capture cross section. In scattering theory, scattering cross section is a measure of the interaction strength. *Interaction* is the key word. Thus, the scattering cross section, or capture cross section in our case, is not the property of a particle or a defect. Rather, it is an indication of the strength of interaction, or in our case the efficiency of the capture process. The value of the cross section must then depend on the specifics of the process, such as $\Delta E$ during capture. Thus, our conclusion that the capture cross section is not a characteristic of an interface defect state can also be generalized to non-interface states, e.g., bulk traps.

Using a kinetic variation of the charge-pumping technique and an argument based on transition-state theory, we have seen how capture cross section is extremely sensitive to how it is measured, and that it does not provide meaningful insight into the physics involved. The capture cross section is not a unique property of an interface defect and thus, there is no need for assigning a cross section value to an interface defect. The concept of capture cross section has led to widespread confusion in the semiconductor device community and has been abused too often as a fudge factor. Its use should be avoided.

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