# Determining the Energy Distribution of Traps in Insulating Thin Films Using the Thermally Stimulated Current Technique

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We have developed a simple method to analyze and predict the thermally stimulated current (TSC) of charged insulating thin films experiencing *arbitrary* time-dependent thermal environments and high electric fields. The method allows greater flexibility in experimental conditions than previous work, and includes the effect of field-induced barrier lowering on the trap energy scale. Trap distributions for irradiated metal-$SiO_2$-Si capacitors were accurately determined from TSC measurements spanning a factor of 50 in heating rate, providing an improved estimate of trapped-hole energies in $SiO_2$ (peak $\sim 1.8$ eV).

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The trap density in energy of insulating thin films is often characterized using the thermally stimulated current (TSC) technique [1,2]. Inferring the trap density in energy from TSC data requires one to compute the trap energy being probed as a function of the thermal history. The intractable nature of the equations describing the relevant mechanisms makes the computations difficult. In an effort to address this problem, Simmons and co-workers developed an approximate solution for the special case of thermal environments with constant ramp rates [1]. Unfortunately, the temperature often does not increase linearly throughout an entire TSC measurement, especially for the high average ramp rates often required to achieve acceptable signal-to-noise ratios. Even if the temperature is increased at a constant rate, the energy scale of Simmons and co-workers can be in error during the early portion of the ramp since it does not take into account the inevitable loss of charge due to traps that are emptied before the ramp is initiated. Finally, the impact of field-induced barrier lowering on the analysis of TSC data has not been extensively investigated.

In this Letter we present a first-principles approach to determine the density of occupied charge traps as a function of trap depth from TSC data obtained using very general environmental conditions. Our method permits the quantitative mapping of temperature to energy using *arbitrary* time-dependent thermal environments, such as those that occur in actual TSC experiments. It also permits the quantitative treatment of the effects of the electric field on TSC data. The present results are directly applicable to thin films in the high field (negligible retrapping) limit. The trap density in energy of radiation-induced holes trapped in a $SiO_2$ film is determined to demonstrate the technique. The trap density is then used to *predict* the thermally stimulated current for a variety of experimental thermal conditions and applied biases, which heretofore has not been possible.

The dielectric films under considerations are assumed to contain charge in traps with some arbitrary distribution of energies. The number density of occupied traps as a function of energy $\phi$ and time $t$ is signified by the function $n(\phi,t)$, which has units of number per unit area per unit energy. It is assumed that the charge leaves the traps by an activated process that can be described by the generalized activation differential equation [3] (with negligible retrapping)

$$\frac{\partial}{\partial t}n(\phi,t) = -n(\phi,t)F(t)\exp\left[-\frac{\phi - R(t)}{A(t)}\right]. \qquad (1)$$

The activation function is $A(t) = kT(t)/q$, where $k$ is the Boltzmann constant, $-q$ is the electronic charge, and $T(t)$ is the time-dependent temperature. In the presence of field-induced barrier lowering, $R(t) = \beta\sqrt{E(t)}$, where $E(t)$ is the time-dependent electric field. For Poole-Frenkel barrier lowering [4] in $SiO_2$, $\beta = \beta_{PF} = (q/\pi\varepsilon)^{1/2} = 3.8\times10^{-5}\ V(V/m)^{-1/2}$; for Schottky emission [5], $\beta = \beta_S = \beta_{PF}/2$ [6]. The function $F(t)$ in Eq. (1) is given by [7,8] $F(t) = a[T(t)]^2$, where $a = 2\sqrt{3}(2\pi)^{3/2}gm^* \times\sigma_t k^2/h^3$, $g$ is the multiplicity of states, $m^*$ is the effective mass of the carriers in the dielectric, $\sigma_t$ is the capture cross section of the dielectric traps, and $h$ is Planck's constant. Using $m^* \approx m_e$, $g \approx 1$, and $\sigma_t \approx 10^{-13}$ cm$^2$ [8-10], we find that $a \sim 3\times10^8\ K^{-2}s^{-1}$ [11].

The general solution to Eq. (1) has recently been extensively developed [3]; here we present only the results relevant to the current analysis. A characteristic energy, signified by the function $q\phi_m(t)$, naturally results from the analysis of Eq. (1). This energy corresponds to the trap depth at which the maximum rate of emission of charge out of traps occurs [1,3,7]. The function $\phi_m(t)$, called the emission front, increases monotonically with time, and is defined as the solution to [3]

$$1 = \int_{t_0}^{t} \frac{A(t)}{A(t')}F(t')\exp\left[-\frac{\phi_m(t) - R(t')}{A(t')}\right]dt'. \qquad (2)$$

Essential to our ability to analyze TSC data is the ability to solve Eq. (2) for $\phi_m(t)$. A technique to easily compute $\phi_m(t)$ for *arbitrary* time-dependent thermal and/or electric field environments has been developed and discussed elsewhere [3], and is not reproduced here.

Consider now, for example, the case of radiation-induced charge trapped in the $SiO_2$ layer of a metal-

$SiO_2$-Si (MOS) structure. Because radiation-induced holes typically are trapped near the Si-$SiO_2$ interface [9,10], it can be shown using Ref. [3] that the initial occupied trap density in energy is given by

$$qn(\phi_m(t),t_0)\approx J(t)\left[\frac{d}{dt}\phi_m(t)\right]^{-1}, \tag{3}$$

provided the trap density does not vary by more than a factor of 2 over a range in energy of $\sim 2kT$. [If the charge is distributed through the dielectric, Eq. (3) contains an extra constant multiplicative term on the right-hand side.] By experimentally measuring the current density $J(t)$ as the traps are depopulated, e.g., by ramping the temperature under bias, and calculating $d\phi_m(t)/dt$ [from Eq. (2) [3]], Eq. (3) can be used to experimentally determine the trap density at the energy $q\phi_m(t)$. Once $n(\phi,t)$ is determined, Eq. (3) is inverted to *predict* the TSC density for other environmental scenarios [12,13]. All that is required is the calculation of $d\phi_m(t)/dt$ for the new experimental conditions. We emphasize that this technique is not restricted to any specific environment; it permits analyses for arbitrary time-dependent thermal or field environments for which negligible retrapping occurs.

To illustrate the analysis, TSC experiments were performed on capacitors consisting of a 350-nm film of $SiO_2$ that separates an *n*-type silicon substrate from a degenerately doped polycrystalline-silicon gate electrode. Holes are introduced and trapped in the $SiO_2$ film by irradiating the capacitor structure with 10-keV x rays under positive bias (gate positive relative to silicon). This method results in holes being trapped in the $SiO_2$ film near the Si-$SiO_2$ interface [9]. A negative voltage is applied to bias the silicon into inversion during the TSC measurement. The emitted charge is thus swept by the internal field to the gate electrode. It is assumed that no charge transport occurs through the Si-$SiO_2$ interface [13]. Additional details regarding sample preparation and the TSC data acquisition system are discussed elsewhere [13].

Here we report four separate TSC experiments performed sequentially on the same sample, but using different temperature ramp rates. In each experiment, charge was introduced by irradiating the sample to a total dose of 6 krad ($SiO_2$) while a bias of +30 V was applied. The TSC measurements were performed with an applied bias of −40 V. To determine the trap density from the TSC data, the electric field must be known. Though the field in the $SiO_2$ varies with both position and time during a TSC measurement, in our analyses we approximate the effect of the field on barrier lowering by using a single effective value for the entire spatial extent of the radiation-induced charge distribution. The effective field we choose is the maximum field, which occurs at the edge of the charge distribution. For our bias configuration, this time-independent field is given approximately by $E\sim V_g/d$, where $V_g$ is the gate bias and $d$ is the dielectric thickness [14]. The initial occupied trap distribution was determined using Eq. (3) with $a\sim 3\times 10^8\ K^{-2}s^{-1}$, $\beta=\beta_S$ (justification will be given later), and the experimentally measured values of the current and temperature for experiment No. 1. The resulting trap density is shown in Fig. 1. The normalized quantity $qn(\phi,t_0)/\sigma_{total}$ is plotted on the vertical axis, where $\sigma_{total}$ is the TSC current density integrated over the duration of the experiment. Since $\sigma_{total}\approx 2.2\times 10^{-7}\ C/cm^2$ for experiments No. 1 through No. 4, one unit on the vertical scale corresponds to $\sim 1.4\times 10^{12}$ charges/(eV cm$^2$).

The measured sample temperature as a function of time is plotted in the inset of Fig. 1 for each TSC experiment. The variation in the ramp rate during the early portion of each experiment requires the ability to treat arbitrary heating conditions to perform quantitative analyses of the full TSC curves. Note that by the time the temperature ramp started (several minutes after the irradiation), $q\phi_m(t)$ had already advanced to $\sim$1.1 eV. To map the trap density at lower energies requires either a change in the early environment (such as lowering the irradiation temperature) to reduce the rate at which $\phi_m(t)$ increases with time, or accurate current measurements earlier in time. Also, quantitative analysis at times on the order of the duration of the irradiation necessitates addressing the charge that is annealing *during* the irradiation.

Using the trap density shown in Fig. 1, the thermally stimulated current as a function of temperature was com-

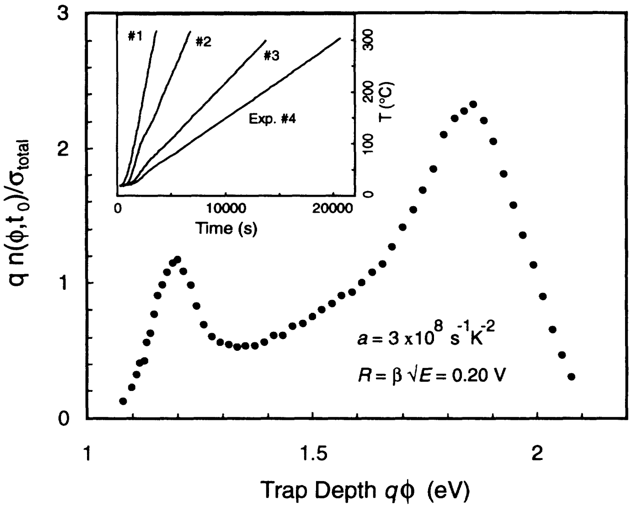

FIG. 1. The normalized radiation-induced-hole trap density $qn(\phi,t_0)/\sigma_{total}$, where $\sigma_{total}$ is the total TSC charge density, is a double-peaked function that drops to $\sim$0 at energies greater than $\sim$2.1 eV above the valence band. Inset: Heating conditions for experiments No. 1 through No. 4. Note that thermal environments for TSC experiments typically are not linear functions of time for the entire TSC ramp.

puted for each environment shown in the inset. The only thing that was changed for the four calculations was the thermal environment. Comparisons of the theoretical results and the experimental data are shown in Fig. 2. Since the trap density was actually determined from experiment No. 1, those TSC data are regenerated by the computation (a self-consistency check of the model). The entire TSC curves for experiments No. 2 through No. 4 are accurately *predicted* from the *single* trap energy distribution. We note that if the value of the constant $a$ was in error by more than an order of magnitude, the TSC curves would not have been predicted as accurately. In particular, the locations in temperature of the peaks would have been in error by $\sim 10\,^{\circ}\mathrm{C}$. Our assumption that $\sigma_t \approx 10^{-13}$ cm$^2$, resulting in $a \approx 3\times 10^{8\pm 1}$ K$^{-2}$s$^{-1}$, is thus supported. Note that the term $F = aT^2$, identified by some as the "attempt-to-escape" frequency, has the rather high value of $\sim 10^{14}$ Hz at 300 °C. This value suggests that optical phonons may contribute to the charge emission process. We also note that the energy scale for the trap density in Fig. 1 differs significantly from that previously inferred for trapped holes in SiO$_2$ using thermal techniques [9,13,15]. Our results are more consistent with trap depths determined by other techniques [9], and are a direct consequence of our more complete treatment of field-induced barrier lowering and the attempt-to-escape frequency [7].

TSC measurements were also made for devices with significantly different oxide trapping characteristics. The trap distributions computed from these measurements, using nonconstant ramp rates spanning a factor of $\sim 50$ (0.25 to 0.0049 K/s), differed from one another by no more than $\sim 0.05$ eV at any energy [16]. Taken together with the data of Figs. 2 and 3 (below), this strongly supports our model of the trapped-hole emission process in SiO$_2$.

A TSC experiment was then performed on a similarly fabricated sample to examine the effects of the bias applied during the TSC measurement. The applied bias for experiment No. 5 was $-70$ V, nearly a factor of 2 greater than the experiments of Fig. 2. The current was predicted using the trap density shown in Fig. 1, and the same values for $a$ and $\beta$. The only changes in the model parameters were the applied voltage and the experimentally measured thermal environment. Figure 3 shows both the theoretical prediction (dashed line) and the experimental data (open circles). Some discrepancy between the model prediction and the experimental data is not unexpected, since the actual occupied trap density in this sample may be subtly different, and our treatment of the barrier lowering field is only approximate. Nevertheless, the higher temperature ($T > 75\,^{\circ}\mathrm{C}$) portion of the TSC curve is predicted remarkably well. Note in particular that this increase in bias (field) shifts the TSC features to a lower temperature (major peak at $\sim 225\,^{\circ}\mathrm{C}$) compared to experiment No. 1 in Fig. 2 (same thermal environment; major peak at $\sim 250\,^{\circ}\mathrm{C}$). The apparent error in predicting the low-temperature peak is simply a result of our approximating the barrier-lowering field by the (constant) maximum field in the dielectric. Reducing the barrier lowering from $R = 0.27$ V to $R = 0.24$ V (a change of only 30 mV) leads to the prediction given by the solid curve. Note that the broadening and reduction in height of the low-temperature peak in Fig. 3 (as compared with experiment No. 1 of Fig. 2) cannot be predicted using the approach of Simmons and

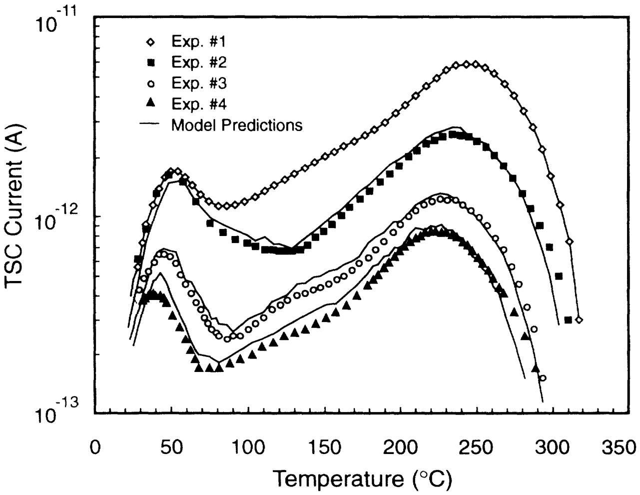

FIG. 2. The experimental TSC curves are accurately predicted by the model with no adjustable fitting parameters. Predictions are made using the measured thermal environments and trap density shown in Fig. 1, and with the values of $a$ and $\beta$ given in the text.

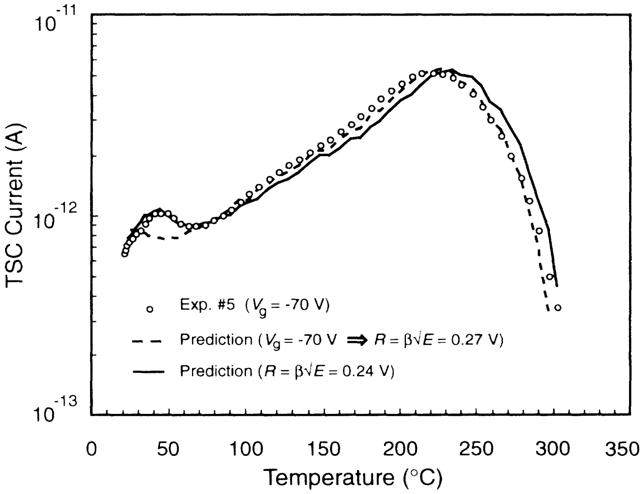

FIG. 3. Using the trap density in Fig. 1 with $R = \beta_S\sqrt{E} = 0.27$ V, the model accurately predicts the experimental TSC data at high temperatures. A reduction in $R$ by 30 mV to $R = 0.24$ V results in the distortion of the low-temperature peak (due to the higher field) being accurately predicted.

co-workers [1]. This seemingly nonintuitive result is in fact a straightforward consequence of the convolution of the nonlinear dependence of $\phi_m$ on $T$ at low temperatures with the shift in energy associated with the barrier lowering. We note also that the results are predicted using the Schottky value $\beta = \beta_S$; the data are *not* predicted using the Poole-Frenkel value $\beta_{PF}$. It has been noted previously that the mechanism of Poole-Frenkel barrier lowering can result in the effective value of $\beta$ being different from the value $\beta_{PF}$ given earlier [17], and can actually be the same as that for Schottky emission [6]. Regardless of the specific mechanism, it is clear that the observed barrier lowering has the same general form as Schottky emission.

Several results suggest that the trap distributions determined by this analysis technique are physically correct. The agreement between model predictions and experimental data for a range of biases (shift and distortion of the TSC curve are predicted) and a range of thermal environments (even subtle features of the TSC curves are predicted) is striking. Also, no adjustable "fitting" parameters are used. If the physically derived parameters $a$ or $\beta$ were significantly in error, the inferred distribution would not be physically correct, and accurate predictions would not result.

In summary, we have developed the capability to compute the trap energy being probed as a function of time for *arbitrary* time-dependent thermal and field environments in the high-field (negligible retrapping) limit. We demonstrated this capability by computing the radiation-induced occupied hole-trap density in energy for an MOS structure from TSC data. This trap distribution was then used to *predict* the thermally stimulated current for a wide range of time-dependent thermal environments and bias conditions. The accuracy of the predictions strongly supports our model assumptions for the wide range of parameters investigated. The results indicate the barrier lowering mechanism for holes in $SiO_2$ is of the same form as Schottky emission. The attempt-to-escape frequency has a value of $\sim 10^{14}$ Hz, suggesting that the emission process may be associated with optical phonons.

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