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Theory of charging and charge transport in “intermediate” thickness dielectrics and its implications for characterization and reliability

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Thin film dielectrics have broad applications, and the performance degradation due to charge trapping in these thin films is an important and pervasive reliability concern. It has been presumed since the 1960s that current transport in intermediate-thickness (IT) oxides (~ 10 – 100 nm) can be described by Frenkel-Poole (FP) conduction (originally developed for $\sim$ mm-thick films) and algorithms based on the FP theory can be used to extract defect energy levels and charging-limited lifetime. In this paper, we review the published results to show that the presumption of FP-dominated current in IT oxides is incorrect, and therefore, the methods to extract trap-depths to predict lifetime should be revised. We generalize/adapt the bulk FP current conduction model by including additional tunneling-based current injection. Steady state characteristics are obtained by a flux balance between contacts and the IT oxide. An analytical approximation of the generalized FP model yields a steady state leakage current $J \propto \exp(-B\sqrt{E})(1 - C\sqrt{E} - D/E)$, where B , C , and D are material-specific constants. This reformulation provides a new algorithm for extracting defect levels to predict the corresponding charging limited device lifetime. The validity and robustness of the new algorithm are confirmed by simulations and published experimental data. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.3691962>]

I. INTRODUCTION

The role of an ultra-thin sub-2 nm gate dielectric for modern integrated circuits is well known,¹ and so is the historical importance of thick dielectrics for wide-ranging applications in electrical insulation.² Interestingly, thin film dielectrics with intermediate thicknesses of ~ 100 nm are also finding important applications in emerging technologies such as radio frequency micro-electro-mechanical systems (RF-MEMS),³ ferroelectric random access memories (FeRAMs), ferroelectric field-effect transistors (FeFETs),⁴ amorphous-silicon-based thin-film solar cells,⁵ and organic electroluminescent devices.⁶ These dielectrics are usually deposited using chemical or physical vapor deposition (CVD or PVD)⁷ techniques. Unlike CMOS technology, where a very high-quality dielectric (SiO_2) is grown thermally over a crystalline silicon substrate,⁸ the PVD- and CVD-deposited dielectrics have higher bulk defect density, due to imperfections in atomic bonding. These defects act as charge trap centers,^{9–12} and during the course of operation of the associated devices, electrons and holes injected from the contacts get trapped in these defects. These time-dependent, stochastic charging and discharging processes in the dielectrics lead to anomalous behavior in device operation, resulting in parametric degradation phenomena, such as shift in capacitance-voltage (CV) characteristics, that leads to stiction in RF-MEMS,¹³ hysteresis loss in ferroelectric dielectrics,¹⁴ efficiency degradation in thin-film solar cells,¹⁵ and charge loss in flash memories.¹⁶

Reliability modeling for these intermediate-thickness (IT) dielectrics depend sensitively on the physical model assumed and the associated parameters (*e.g.*, trap depth, trap density, effective mass, etc.) used to interpret the temporal evolution of trapped charges within the dielectric. This sensitivity is illustrated in Fig. 1, where we plot (using the model proposed by Melle *et al.*¹⁷) the calculated rate of change of actuation voltages for a typical RF-MEMS capacitive switch due to trapped charges as a function of stress bias applied to the dielectric. The degradation rates vary by orders of magnitude for small variations in the dielectric trap depth. It is therefore important to characterize the parameters accurately and to cross-check for consistency with complementary experiments.

FIG. 1. (Color online) Simulated variation of shift-rate of actuation voltages (SRAV) for a RF-MEMS device as a function of stress electric field on the dielectric. Different dielectric trap depths lead to very different SRAVs.

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The various parameters of a dielectric have historically been extracted by interpreting the steady state leakage characteristics (current-voltage – I - V) by appropriate physical models. For example, the parameters of very thin dielectrics (< 5 nm) are obtained by interpreting the leakage current by assuming Fowler-Nordheim (FN)- or direct tunneling¹⁸-dominated transport, while those for very thick dielectrics (> 1 μ m) are obtained by assuming Frenkel-Poole (FP)-dominated conduction (see Fig. 2). In thin dielectrics, the tunneling of charge carriers between the contacts dominates total leakage. In contrast, in very thick dielectrics, the leakage current is limited by emission and capture rates in the bulk of the dielectric, rather than by the fill rate of traps from the contacts. Therefore, carrier transport in thick films is relatively insensitive to the contacts and dominated by bulk properties of the corresponding dielectrics. Hence, it is easy to justify the use of FP transport to interpret results for thick dielectrics,¹⁹ and this was precisely the original intent of the theory developed in 1930s.²⁰

Over the years, the FP conduction has been used for fitting experimental I - V characteristics for progressively thinner dielectrics (without taking into account the trapping dynamics near the contacts), and there has been very little discussion if the use of FP leakage is justified when the oxide thickness reaches ~ 10 s of nm, i.e., the “intermediate thickness” regime. In Fig. 3(a), we summarize the current-density–electric field (J - E) characteristics for different dielectrics of thicknesses between 10 nm and 30 nm.^{21–24} It may appear initially that the FP assumption is justified, since the FP plots ($\log(J/E) \propto \sqrt{E}$) appear essentially linear. On closer inspection, however, we find the slope of the curve depends strongly on E (Fig. 3(b)), whereas one expects the slope to be constant if the current is dominated by FP conduction (at least for some range of values of E). Furthermore, there have been disagreements on whether it is the leakage current density (J) or the conductivity (J/E) that should be proportional to $\exp(\sqrt{E})$.²⁵ Attempts to extract trap-depth

FIG. 2. (Color online) Schematic band-diagrams of dielectrics of different thicknesses under a stress voltage. The dotted line inside the band-gap represents the spatially distributed trap level. In very thin dielectrics, charge carriers can tunnel directly through the dielectric (Fowler-Nordheim (FN) or direct tunneling) or via the traps (trap-assisted tunneling). In very thick dielectrics, on the other hand, the Frenkel-Poole (FP) emission process is the rate-limiting step and determines leakage current behavior. In the intermediate thickness regime, both processes of trap-filling by tunneling as well as trap-emptying by emission will compete, and the leakage current is expected to be different from those of very thin or very thick dielectrics.

FIG. 3. (Color online) (a) Current density vs. electric field (J - E) characteristics for several different thin-film dielectrics of various thicknesses obtained from published literature (Refs. 21–24). (b) Slope of the Frenkel-Poole curve ($\log(J/E)$ vs. $\sqrt{E}$) for each set of curves in (a). The variability of the slope makes the exclusive use of FP conduction model questionable.

assuming FP leakage behavior, therefore, are likely to yield unphysical dependence on the electric field. Such discrepancies regarding applicability of FP assumption to dielectric leakage currents have been reported in the recent past²⁶ and have generally been attributed to an unspecified “anomalous” FP conduction mechanism.²⁷

Given these limitations of the classical FP model for intermediate thickness dielectrics, several other techniques have been used to characterize trap-depths and trap densities in dielectrics,^{28–32} including deep level transient spectroscopy (DLTS)³³ and impedance/admittance spectroscopy (IS)³⁴ for semiconductors and/or low band-gap materials. These techniques often require the use of sophisticated measurement equipment and/or transistor structure for characterization. Furthermore, the DLTS and IS are rendered ineffective in the characterization of higher band-gap materials, like silicon nitride (Si_3N_4), zirconium oxide (ZrO_2), aluminum nitride (AlN), or aluminum oxide (Al_2O_3), all of which are routinely used in thin-film technologies.

In this paper, we discuss in Sec. II a theoretical modeling framework for charge trapping/detrapping dynamics in intermediate thickness (IT) dielectric films in a metal-insulator-metal (MIM) capacitor structure (see Fig. 4). In this new

FIG. 4. (Color online) (a) Schematic diagram of a generic metal-insulator-metal (MIM) system. (b) Band diagram of the MIM system shown in (a). Dielectric thicknesses and voltage applied across the dielectric is indicated in both (a) and (b). The defects in the dielectric trap charges over a period of time during the course of operation of the device, leading to reliability issues. Circles marked negative are trapped electrons and those marked positive are trapped holes.

approach, we generalize the FP model to include both trap-assisted tunneling as well as FP capture/emission processes, and bridge the gap between the two seemingly different conduction domains of very thin and very thick dielectrics. The full model can only be solved numerically; however, we show in Sec. III that, with a few simplifying assumptions, one can develop a compact analytical expressions for the steady-state trap-assisted leakage currents for a dielectric under given operating conditions. We demonstrate that the steady state leakage currents reported in the published literature do not follow the classical FP conduction mechanism, and therefore, the trap-depths extracted using the FP assumption are potentially incorrect. We suggest in Sec. IV an improved algorithm to extract trap properties in the dielectric. Our conclusions are summarized in Sec. V.

II. THEORY AND MODEL

The band-diagram of a typical MIM capacitor (Fig. 4(a)) is shown in Fig. 4(b). We assume the following to model charging dynamics of the MIM capacitor:

- Since the cross-sectional area of a typical MIM system is significantly larger than the dielectric thickness, the electric field inside the dielectric is essentially one dimensional. Consequently, for simplicity, the trapping/detrapping dynamics are also assumed one dimensional, although the generalization to 3D is conceptually straightforward.
- For many metal-dielectric interfaces,³⁵ the offset of the conduction band is smaller than that of the valence band. The conduction in these insulators is thus dominated by electron injection and transport rather than by holes; therefore, in the following discussion, for simplicity, we consider only electron transport. The model can be generalized to include hole transport, if necessary.
- We assume that the band-bending of the contact Fermi level near the metal-dielectric interface is negligible, because electron densities in the metal is high and screening length is extremely short screening lengths. For semiconductor-insulator boundaries, however, one must account for the associated band-bending in the semiconductor.
- We use an effective mass model for electrons in tunneling calculations. Here, the effective mass (m^*) is treated as an empirical parameter, because it is difficult to include exact band-structure information associated with amorphous dielectrics.³⁶
- Traps are distributed uniformly inside the dielectric bulk with a given trap density (N_T) and a field-independent capture cross section (σ). Generalization to non-uniform spatial distributions of traps is easily implemented in the model.
- Electron capture into the traps is assumed to be phonon assisted. If the electron's original energy is higher than the trap energy, the electron is captured with probability 1; otherwise, the probability reduces exponentially with the difference between the energy levels. The model is easily generalized to include activated capture.
- We neglect the relaxation in trap energy (due to atomic reconfiguration) following electron capture. Again, the modification of the model to include such relaxation is straightforward.

The trap level is indicated by a dashed line inside the band-gap (Fig. 5). The electron barrier height (Φ_B) is defined as the energy difference between the contact work function (Fermi level) and dielectric conduction band. Both Φ_B and the trap depth (Φ_T) have been marked in the figure. Although the complete solution of charge carrier transport and dynamics has been considered and solved for (discussed in Appendix A), we identify three dominant electron trapping/de-trapping mechanisms for further discussion in this section. These include electron injection from the metal contact (M_2) into the traps by tunneling (current flux: J_{IN}), electron leakage from the traps into M_2 (current flux: J_{OUT}), and electron emission from the traps into dielectric conduction band (current flux: J_E). The variables and parameters used to formulate the model are summarized in Table I.

The density of occupied traps at position x and at time t is given by $n_T(x, t)$. We discretize the dielectric in x with a grid spacing of Δx . The metal Fermi level of the contact at $x=0$ is treated as a reference energy level, and all other energy values (E) are calculated with respect to this reference. Other constants being used are the elementary electronic charge (q), the free electron mass (m_e), Planck's constant (h), Boltzmann's constant (k_B), and permittivity of free space (ϵ_0).

The electron flux from the metal contacts into a trap located at distance x from the contact— $J_{IN}(x, t)$ —is given by a modified Tsu-Esaki formula,³⁷

$$J_{IN}(x, t) = \frac{4\pi m^* q}{h^3} \sigma \Delta x [N_T - n_T(x, t)] \times \int_{-\infty}^{\infty} T^r(E, x) \beta_1(E, x) S(E) f(E) dx, \\ J_{IN}(x, t) \equiv A_{IN}(x) [N_T - n_T(x, t)]. \quad (1)$$

The factor $\sigma \Delta x [N_T - n_T(x, t)]$ in Eq. (1) denotes the ratio of the effective capture area of all the empty traps inside a

FIG. 5. (Color online) The trapping-detrapping current mechanisms (J_{IN} , J_{OUT} , and J_E) considered in this study are marked on the band-diagram along with the trap-depth (Φ_T) and barrier height (Φ_B).

TABLE I. List and description of all dielectric parameters used for modeling leakage currents and trap occupancies.

Symbol	Units	Description
V	V	Applied voltage
T	K	Ambient temperature
N_T	m^{-3}	Total trap (defect) density
n_T	m^{-3}	Density of occupied traps
T_d	m	Dielectric thickness
ϵ_r	...	Dielectric constant
Φ_B	eV	Barrier height
Φ_T	eV	Trap depth
σ	m^2	Capture cross section
m^*	Kg	Electron effective mass
γ	s^{-1}	FP attempt frequency
ϵ_∞	...	Optical dielectric constant

region of width Δx within the insulator to the total cross-section of the metal-insulator contact interface. In general, the capture cross-section σ can be field-dependent and temperature-activated.^{38,39} The elastic tunneling transmission probability, $T^r(E, x)$, describes tunneling of electrons from the metal contact to a distance x into the dielectric at energy E , calculated using the Wentzel-Kramers-Brillouin (WKB)⁴⁰ approximation to Schrodinger equation for smoothly varying potential barriers; $f(E)$ is the fraction of occupied states in the metal assuming Fermi-Dirac statistics; the supply function $S(E)$ is obtained by integrating the Fermi function over the transverse energy component of electrons inside the metal;³⁷ and $\beta_I(E, x)$ is the inelastic scattering probability of an electron between the tunneling and the trap energy levels, calculated based on assumption (g). Expressions for $T^r(E, x)$, $f(E)$, $S(E)$, and $\beta_I(E, x)$ are given in Appendix A (Eqs. (A1)–(A4)). Note that, in Eq. (1), the term $A_{IN}(x)$ has been used to separate out trap occupancies from the other terms.

The expression for the current flux of trapped electrons inside the insulator leaking out to empty states in the metal by tunneling— $J_{OUT}(x, t)$ —is expressed by modifying Eq. (1),

$$J_{OUT}(x, t) = \frac{4\pi m^* q}{h^3} \sigma \Delta x [N_T(x, t)] \times \int_{-\infty}^{\infty} T^r(E, x) \beta_2(E, x) S(E) (1 - f(E)) dE, \\ J_{OUT}(x, t) \equiv A_{OUT}(x) [N_T(x, t)]. \quad (2)$$

The term $1 - f(E)$ is the fraction of empty states in the metal for electrons tunneling at energy E . The inelastic scattering probability function $\beta_2(E, x)$ is different compared to $\beta_I(E, x)$, because the values of initial and final energy levels are reversed.

The trapped electrons escape the traps into the dielectric conduction band via an electric-field-assisted, temperature-activated Frenkel-Poole (FP) emission process.^{20,41,42} The electric field reduces the effective trap-depth by $\Delta\Phi_T$, increasing the thermal emission rate for trapped electrons. The expression for FP emission flux— $J_E(x, t)$ —is given by

$$J_E(x, t) = \gamma q \Delta x [n_T(x, t)] \exp \left(- \frac{\Phi_T - \sqrt{\frac{q^3 \mathbf{E}(x)}{\pi \epsilon_0 \epsilon_\infty}}}{k_B T} \right) \\ J_E(x, t) = \gamma q \Delta x [n_T(x, t)] \exp \left(- \frac{\Phi_T - \beta \sqrt{E}}{k_B T} \right) \\ \equiv A_E(x) [n_T(x, t)]. \quad (3)$$

The optical dielectric constant of the dielectric (ϵ_∞) in Eq. (3) is equal to n^2 , where n is the refractive index. The electrons emitted out of the traps are free to move in the conduction band, subject to drift and diffusion. These electrons could be repeatedly captured into other trap locations and re-emitted to the conduction band until they exit through either of the metal contacts.

III. DERIVING THE COMPACT MODEL

The current flux $J_{IN}(x, t)$ fills the traps, and fluxes $J_{OUT}(x, t)$ and $J_E(x)$ empty the traps, as discussed in Sec. II. For the derivation of the compact model, we assume that emitted electrons are swept away to the metal contact by the electric field. In reality, these electrons are subject to drift-diffusion transport in the conduction band and may be recaptured multiple times into traps in the dielectric. This multiple trapping/emission effect has been accounted in the complete numerical framework developed and discussed in Appendix A. We subsequently justify, in Appendix B, the assumptions made in the following derivation of the compact model (i.e., electric field within the dielectric is essentially constant and that the drift-diffusion process in the conduction band and recapture of electrons from conduction band are not the rate-limiting processes of the conduction problem, etc.). We frequently use the results from the numerical solution for the IT oxides as a reference for other approximate solutions to charge-trapping dynamics. The compact model thus developed will be used to determine the defect levels in Sec. IV—a key goal of the paper.

To obtain the rate of change of trap occupancy at a given position x and time t , Eqs. (1), (2), and (3) can be combined to yield a first-order differential equation,

$$q \Delta x \frac{dn_T(x, t)}{dt} = J_{IN}(x, t) - J_{OUT}(x, t) - J_E(x, t), \\ q \Delta x \frac{dn_T(x, t)}{dt} = A_{IN}(x) N_T - A(x) n_T(x, t), \quad (4)$$

where $A(x) = A_{IN}(x) + A_{OUT}(x) + A_E(x)$.

Equation (4) is the continuity equation for the traps and accounts for charge conservation. This continuity equation can be solved for trapped charge densities at position x and time t ($n_T(x, t)$) as well as the transient leakage current $J(t) = \sum_x (J_{IN}(x, t) - J_{OUT}(x, t))$. However, in this paper, we confine ourselves to steady state response, obtained by calculating $\lim_{t \rightarrow \infty} J(t)$ as follows:

$$J_S = \sum_x \frac{A_{IN}(x) A_E(x) N_T}{A(x)}. \quad (5)$$

This formulation suggests that, depending on the nature of the dielectric, either electron injection from the contacts

(J_{IN}) or FP-based electron emission from the traps (J_E) can act as the rate-limiting process. It is therefore easy to understand why a model that relies exclusively on FP conduction might fail to predict trap levels in IT oxides in a general case.

Equation (5) can be simplified to yield a compact form for the steady state leakage current (detailed derivation leading the compact model is described in Appendix B). It is observed from numerical simulations that, for high electric fields, leakage current contribution from region R_2 exceeds that from region R_1 (see Fig. 11 in Appendix B). Since $J_{S-R1} \ll J_{S-R2}$ and $J_S = J_{S-R1} + J_{S-R2}$, therefore, $J_S \approx J_{S-R2}$. The expression for J_S (from Eq. (A18) in Appendix B) can therefore be approximated for high E as follows:

$$J_S = q\gamma N_T \exp(-\chi) \left[\frac{1}{\eta} \log\left(\frac{\alpha_{IN}}{q\gamma}\right) + \frac{\chi}{\eta} - x_1 \right]. \quad (6)$$

From numerical simulations, we find that the first term inside the square bracket can be neglected under typical operating conditions. After eliminating the first term and substituting the values for x_1 and χ (Eqs. (A9) and (A17) in Appendix B), we rewrite Eq. (6) as follows:

$$J_S = q\gamma N_T \exp\left(-\frac{\Phi_T - \beta\sqrt{E}}{k_B T}\right) \left[\frac{\Phi_T - \beta\sqrt{E}}{\eta k_B T} - \frac{\Phi_B - \Phi_T}{qE} \right],$$

or, equivalently, as

$$J_S(E) = \frac{q\gamma N_T \Phi_T}{\eta k_B T} \exp\left(-\frac{\Phi_T - \beta\sqrt{E}}{k_B T}\right) \times \left[1 - \frac{\beta\sqrt{E}}{\Phi_T} - \frac{\Phi_B - \Phi_T}{qE\Phi_T} \eta k_B T \right], \quad (7)$$

where $\eta \equiv \frac{2\sqrt{2m^* \Phi_B}}{\hbar}$.

Equation (7) is the key result of this paper. It is immediately obvious that Eq. (7) for leakage currents differs from the widely accepted FP conductivity model by several correction factors. The fact that the leakage current through thin film dielectrics cannot be described by FP-like transport has already been demonstrated in Fig. 2. Since extraction of other dielectric parameters, such as ϵ_∞ and Φ_T , depend on the accuracy of the transport model, the generalized FP-like formula of Eq. (7) will improve dielectric parameter extraction. In Sec. IV, we validate this hypothesis by using Eq. (7) to back-extract dielectric parameters from simulated current-voltage leakage characteristics obtained using Eq. (5), as well as those from published experimental data.

IV. PARAMETER EXTRACTION

Equation (7) can be used to develop the following characterization methodology for dielectric properties, like defect energy levels:

- The expression for $J_S(E)$ is parameterized using parameters **a**, **b**, **c**, and **d** (see Eq. (8) below). One determines these parameters by multiple parameter curve-fitting of Eq. (8) to experimental data in the high- E regime.

$$\log(J_S(E)) = a + b\sqrt{E} + \log\left(1 - c\sqrt{E} - \frac{d}{E}\right), \quad (8)$$

where

$$a = \log\left(\frac{q\gamma N_T \Phi_T}{\eta k_B T}\right) - \frac{\Phi_T}{k_B T}, \quad (8a)$$

$$b = \frac{\beta}{k_B T}, \quad (8b)$$

$$c = \frac{\beta}{\Phi_T}, \quad (8c)$$

$$d = \frac{\Phi_B - \Phi_T}{q\Phi_T} \eta k_B T. \quad (8d)$$

From Eqs. (8b) and (8c)

$$\Phi_T = \frac{bk_B T}{c}. \quad (8e)$$

- One begins by fitting **a** versus $1/T$ using the functional form of Eq. (8a). This gives us the trap-depth Φ_T and the value of $\gamma N_T/\eta$.
- Φ_T is recalculated by using Eq. (8e). If the model being used to fit experimental characteristics (i.e., Eq. (7)) is correct, the value of Φ_T thus obtained should be the same as that obtained in step (b).
- Next, **b** versus $1/T$ is fitted using Eq. (8b) to obtain ϵ_∞ from the slope of the fit. *Note that the fit is expected to pass through the origin.* This property of Eq. (8b) can be used as a constraint to obtain better and physically relevant fitting information.
- Finally, **d** versus T is fitted using Eq. (8d) to obtain $\eta(\Phi_B/\Phi_T - 1)$ from the slope of the fit. Again, similar to step (d), we use the constraint that the fit is expected to pass through the origin to improve parameter extraction.

One observes from Eq. (8e) that the parameters **a**, **b**, **c**, and **d** are not independent. The co-dependencies can be used to check for self-consistency of the extracted parameters. For example, if the values of Φ_T obtained in steps (a) and (c) were different, it would indicate that Eq. (8) is not the right model to apply for leakage current characteristics.

We validate the compact model and the parameter extraction algorithm in two steps, as listed below.

A. Numerically simulated J-E characteristics versus extraction algorithm

We first numerically simulate the charge transport for a model system with a 100-nm silicon nitride (Si_3N_4) dielectric. We assume that the traps are located at 1.3 eV below the dielectric conduction band. Results of the full self-consistent numerical simulation of transport through the film for a broad range of voltages and temperatures are shown in Fig. 10 (in Appendix A), where currents obtained from Eq. (5) are compared against those obtained from full numerical Poisson self-consistent simulations.

Given this numerically synthesized J - E - T data, we use the MATLAB curve-fitting tool (cftool) to determine the constants **a**, **b**, **c**, and **d** of Eq. (8) at each temperature, T . We use

FIG. 6. (Color online) Demonstration of the proposed parameter extraction algorithm from simulated data points obtained by using Eq. (5). In step (a), we observe that the leakage current expression in Eq. (7) fits the simulated data points exactly. Also, the extracted parameters Φ_T , ϵ_∞ , $\gamma N_T/\eta$, and $\gamma(\Phi_B/\Phi_T - 1)$ in steps (b), (d), and (e) are almost equal to the ones used to obtain the simulated data points (indicated in brackets). Note that the fits of b vs $1/T$ in step (d) and d vs T in step (e) must pass through the origin, because of their functional constraints (Eqs. (8b) and (8d)). Also note that the consistency requirement imposed on the model by step (c) is also satisfied, since Φ_T values extracted from step (a) and using Eq. (8e) lie very close to each other.

steps (b)-(d) to back-extract trap-depth Φ_T , optical dielectric constant ϵ_∞ , and values of $\gamma N_T/\eta$ and $\eta(\Phi_B/\Phi_T - 1)$. This process is illustrated in Fig. 6. We observe that the extracted parameters are almost identical to the values used to create the data points based on complete numerical simulation. This indicates that the approximations used to derive Eq. (7) are correct, and therefore, the extraction methodology is valid. Furthermore, the self-consistency required by step (c) is also satisfied, since the two values of Φ_T obtained from Eqs. (8a) and (8b) are equal with a very small error margin. Note that, even though the parameter extraction method is being used on simulated J - E curves, the equations used to generate the simulated data points and to back-extract the parameters are different, and the fact that the extracted parameters are equal to the ones used for data point generation implies the correctness of Eq. (7) and steps (a)-(e) associated with Eq. (8), as discussed above.

B. Experimental J-E characteristics versus extraction algorithm

Having verified the aforementioned parameter extraction process using simulated J - E - T curves, we now demonstrate the validity of the approach by interpreting the measured J - E - T curves for a 10-nm ZrO_2 dielectric obtained from Kwon *et al.*²¹ The results have been summarized in Fig. 7. Using the MATLAB curve-fitting tool for steps (a) and (b), we obtain the desired parameters, as indicated in the insets of plots in Fig. 7. Most importantly, the trap-depth values extracted in step (b) are found to be consistent with those

obtained from the verification step (c), which implies the correctness of Eq. (7) being used for this system.

Even though this extraction methodology does not yield all the dielectric parameters being used in the model individually, it imposes four constraints on the parameter space (values of Φ_T , ϵ_∞ , $\gamma N_T/\eta$, and $\gamma(\Phi_B/\Phi_T - 1)$). This simplifies the process of curve fitting of experimental data to Eq. (5). We use Eq. (5) and values obtained from the parameter extraction process to fit the experimental data and observe a very good match between experimental data points and simulations (see Fig. 8). All the dielectric parameters extracted in this process (tabulated in Table II) are found to lie within acceptable limits. The constraint that the d versus T plot must pass through origin allows us to extract the physically meaningful quantity $\gamma(\Phi_B/\Phi_T - 1)$, even with less than perfect experimental data.

Note that, since the leakage current characteristics do not exhibit FP-like behavior, the dielectric properties extracted using an assumption of “pure FP current transport” are likely to be incorrect. Equation (7) therefore provides a better method of characterizing IT dielectrics.

V. SUMMARY AND CONCLUSIONS

To summarize, in this paper, we have developed a generalized FP model to calculate leakage currents and charge trapping in CVD/PVD-deposited dielectrics. This model calculates the rate of charge accumulation in the dielectric and, subsequently, the leakage currents by balancing the filling and emptying rates for the traps. We find that the leakage

FIG. 7. (Color online) Demonstration of the proposed parameter extraction algorithm from the experimental data (Ref. 21). We follow the same procedure as done for simulated data points in Fig. 6. We observe an excellent fit of Eq. (7) to the data, and the consistency requirement on Φ_T in step (c) is also satisfied. The parameters Φ_T , ϵ_∞ , $\gamma N_T/\eta$, and $\gamma(\Phi_B/\Phi_T - 1)$ have been extracted in steps (b), (d), and (e). Note: The requirement that Eqs. (8b) and (8d) pass through the origin was used in fitting in steps (d) and (e).

FIG. 8. (Color online) Fitting of Eq. (5) to experimental data points using values of Φ_T and ϵ_∞ and values of $\gamma N_T/\eta$ and $\gamma(\Phi_B/\Phi_T - 1)$ extracted by the process demonstrated in Fig. 7. The parameters which are thus extracted and used for the fit have been listed in Table II.

current characteristics of these dielectrics cannot be exclusively described by classical Frenkel-Poole transport, and therefore, any trap-depth values extracted using this assumption may be incorrect. A compact model for leakage current has been developed based on a few well-justified simplifying assumptions. The compact model proposed replicates numerical simulation results accurately, implying the assumptions underlying the compact model formulation are correct. The motivation of extracting the correct dielectric trap-depth has been satisfied by a proposed dielectric parameter extraction procedure using experimental leakage current characteristics based on the compact model. This procedure has been verified using simulation data as well as measurement data from existing literature. The parameters thus extracted are found to lie within well-accepted limits.

The proposed model has several limitations. The model does not account for variation of trap density across the thickness of a dielectric, nor does it account for distribution of trap energy levels across the bandgap; therefore the parameters extracted should be viewed as being effective parameters spatially averaged over the thickness of the film. Moreover, the surfaces of CVD thin films are known to be rough⁴³ and may lead to uneven field distribution and spatially inhomogeneous charge injection into the film.⁴⁴ Therefore, the assumption about one-dimensional electric field may not always be appropriate. In spite of all these limitations, to the best of our knowledge, the modeling approach

described in this work provides an intuitive and comprehensive generalization of the existing models for trapped charge accumulation and current leakage in intermediate thickness dielectrics and offers a robust and improved algorithm for characterization of defect levels and dielectrics constants within such a dielectric.

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APPENDIX A: NUMERICAL SIMULATION

The model discussed in Sec. II of this paper only describes three main current fluxes (J_{IN} , J_{OUT} , and J_E) which contribute to trapping dynamics. Expressions for the WKB elastic tunneling transmission probability $T^r(E, x)$, Fermi-Dirac distribution function $f(E)$, supply function $S(E)$, and scattering coefficient $\beta_1(E, x)$ (discussed in Sec. II) are given by

$$T^r(E, x) = \exp\left(-\frac{2}{\hbar} \int_0^x \sqrt{2m^* (\Phi_B - q\phi(x') - E)} dx'\right), \quad (\text{A1})$$

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)}, \quad (\text{A2})$$

$$S(E) = \int_0^\infty f(E) dE_\parallel = k_B T \log\left(1 + \exp\left(-\frac{E - E_F}{k_B T}\right)\right), \quad (\text{A3})$$

$$\beta_1(E, x) = \begin{cases} 1 & \Delta E < 0 \\ \exp\left(-\frac{\Delta E}{k_B T}\right) & \Delta E \geq 0 \end{cases}, \quad (\text{A4})$$

where $E_\parallel$ is the transverse energy component of the tunneling electrons.

Emitted electrons are assumed to exit the dielectric due to the electric field. In reality, however, the emitted electrons in the conduction band are subject to drift-diffusion transport and can be recaptured by another trap physically located elsewhere in the dielectric. The capture rate— $J_C(x)$ —depends upon the density of electrons in the conduction band— $n_C(x)$ —and the number of empty traps at that position— $[N_T - n_T(x)]$ —and is given by⁴⁵

$$J_C(x, t) = q \Delta x \sigma_C v_{TH} n_C(x, t) [N_T - n_T(x, t)].$$

Here, σ_C is the cross section offered by a trap for electron capture from the conduction band and v_{TH} is the thermal velocity. Now, instead of only one continuity equation for $n_T(x, t)$ (Eq. (4)), we can write two continuity equations for the system for $n_T(x, t)$ and $n_C(x, t)$, separately, as

TABLE II. Values of the parameters used in the fit used in Fig. 8. We see that all the values are within acceptable limits.

Variable	Description	Extracted value
N_T	Trap density	$1.2 \times 10^{24} \text{ m}^{-3}$
Φ_B	Barrier height	1.5 eV
Φ_T	Trap depth	1.18 eV
σ	Capture cross section	10^{-22} m^2
m^*	Effective mass	0.46
γ	FP attempt frequency	$9.2 \times 10^9 \text{ s}^{-1}$
ϵ_∞	Optical dielectric constant	3.18

$$q\Delta x \frac{dn_T(x,t)}{dt} = J_{IN}(x,t) - J_{OUT}(x,t) - J_E(x,t) + J_C(x,t), \quad (\text{A5})$$

$$q\Delta x \frac{dn_C(x,t)}{dt} = J_E(x,t) - J_C(x,t) - J_{D-D}(x,t). \quad (\text{A6})$$

The term $J_{D-D}(x,t)$ in Eq. (A6) is the contribution due to drift-diffusion transport in the conduction band and can be decomposed into a linear combination of $n_C(x - \Delta x, t)$, $n_C(x, t)$, and $n_C(x + \Delta x, t)$. The continuity equations (Eq. (A5), (A6)) are therefore a system of coupled linear differential equations, which can be generally expressed as a matrix equation

$$\frac{d\overline{\mathbf{N}}(t)}{dt} = \mathbf{A}(t)\overline{\mathbf{N}}(t) + \mathbf{D}(t). \quad (\text{A7})$$

Here,

$$\overline{\mathbf{N}}(t) = \begin{bmatrix} n_T(0, t) \\ n_T(\Delta x, t) \\ \vdots \\ n_T(T_d, t) \\ n_C(0, t) \\ n_C(\Delta x, t) \\ \vdots \\ n_C(T_d, t) \end{bmatrix}.$$

Equation (A7) is discretized in time using backward Euler method,

$$\overline{\mathbf{N}}(t + \Delta t) = [\mathbf{I} - \mathbf{A}(t)\Delta t]^{-1} [\overline{\mathbf{N}}(t) + \mathbf{D}(t)\Delta t]. \quad (\text{A8})$$

Equation (A8) is solved numerically for $\overline{\mathbf{N}}(t)$ using the CSparse library for sparse linear systems,⁴⁶ self-consistently with the Poisson equation. This solution process is summarized in the flow chart in Fig. 9. Since the trap occupancies change after each time step, the potential profile in the dielectric changes as well, and therefore, the matrices $\mathbf{A}$ and $\mathbf{D}$ have to be recalculated after each time step. This process makes this simulation approach computationally intensive. However, we see from Fig. 10 that the analytical approximation in Eq. (5) yields very similar results to those obtained from the complete numerical simulations with significantly less computational burden. Contribution due to Poisson self-consistency becomes significant only at high dielectric thicknesses and trap densities. The effect of drift-diffusion and electron recapture is also found to be insignificant. This justifies the assumption that emitted electrons are swept away to the metal contacts by the applied electric field. In Appendix B, we describe how the analytical model in Eq. (5) is simplified further to obtain closed-form expressions for steady state leakage currents.

APPENDIX B: COMPACT MODEL

In this section, the expression for J_S in Eq. (5) may be simplified further to obtain the closed form equivalent in terms of dielectric parameters and applied voltage and tem-

FIG. 9. Flow chart for the Poisson self-consistent solution process to compute trapped charge densities and leakage currents in a trap-filled thin-film dielectric.

perature conditions. To do so, we divide the dielectric into three regions (Fig. 11). It is determined from the numerical simulations that the contribution to J_S from Region 3 (R_3) is small compared to R_1 and R_2 . Therefore, contributions from only R_1 and R_2 are considered in this analysis.

The locations of the boundaries between the different regions (x_1 and x_2) in terms of Φ_T and Φ_B are given by

$$x_1 = \frac{\Phi_B - \Phi_T}{qE} \quad \text{and} \quad x_2 = \frac{\Phi_B}{qE}. \quad (\text{A9})$$

Assuming that most of the injection occurs from the metal Fermi-level, the integration over energy E in Eqs. (1) and (2)

FIG. 10. (Color online) Comparison between steady state leakage current ($J_S(E)$) for Poisson self-consistent numerical simulation (symbols) and the analytical formulation in Eq. (5) (lines) under different operating conditions. Note that the results obtained from the two approaches are almost identical. The compact model (Eq. (7)) yields similar results. This implies that use of the approximations which lead up to the compact model is justified.

FIG. 11. (Color online) The dielectric is divided into three regions R₁, R₂, and R₃ for the purpose of formulating the compact model for charge transport and leakage currents. The boundaries between the regions are determined by trap-depth, barrier height, and electric field (Eq. (A9)).

for $T^r(E, x)$ and $\beta(E, x)$ is removed. To account for the spread in electron density over energy in the metal with temperature, only $S(E)f(E)$ is integrated over E ,

$$\int_{-\infty}^{\infty} S(E)f(E)dE = \frac{\pi^2(k_B T)^2}{6}. \quad (\text{A10})$$

The transmission coefficient $T^r(x)$ (Eq. (A1)) for $E = E_F$ can be simplified by using binomial approximation for the term under the square root as follows:

$$T^r(x) = \exp\left(-\frac{2\sqrt{2m^*\Phi_B x}}{\hbar}\right) = \exp(-\eta x). \quad (\text{A11})$$

This expression holds true for both regions R₁ and R₂, where the electrons tunnel through a trapezoidal barrier. The scattering factors β_1 and β_2 for $E = E_F$ in regions R₁ and R₂ are determined as follows:

$$\beta_1(x) = \begin{cases} \exp\left(-\frac{\Phi_B}{k_B T}\right)\exp\left(\frac{qEx}{k_B T}\right) & \text{in R}_1 \\ 1 & \text{in R}_2 \end{cases}, \quad (\text{A12})$$

$$\beta_2(x) = \begin{cases} 1 & \text{in R}_1 \\ \exp\left(\frac{\Phi_B}{k_B T}\right)\exp\left(-\frac{qEx}{k_B T}\right) & \text{in R}_2 \end{cases}. \quad (\text{A13})$$

Using Eqs. (A10)–(A13), we derive closed form expressions for the coefficients $A_{IN}(x)$, $A_{OUT}(x)$, and $A_E(x)$ (Eqs. (1)–(3) in Sec. II),

$$A_{IN}(x) = \begin{cases} \alpha_{IN}\Delta x \exp(-\eta x + \xi x - \Phi) & \text{in R}_1 \\ \alpha_{IN}\Delta x \exp(-\eta x) & \text{in R}_2 \end{cases}, \quad (\text{A14})$$

$$A_{OUT}(x) = \begin{cases} \alpha_{IN}\Delta x \exp(-\eta x) & \text{in R}_1 \\ \alpha_{IN}\Delta x \exp(-\eta x - \xi x + \Phi) & \text{in R}_2 \end{cases}, \quad (\text{A15})$$

$$A_E(x) = q\gamma\Delta x \exp(-\chi). \quad (\text{A16})$$

Here,

$$\alpha_{IN} = \frac{4\pi m^* q \sigma \pi^2 (k_B T)^2}{h^3}, \quad \xi = \frac{qE}{k_B T}, \quad (\text{A17})$$

$$\Phi = \frac{\Phi_B - \Phi_T}{k_B T}, \quad \text{and} \quad \chi = \frac{\Phi_T - \beta\sqrt{E}}{k_B T}.$$

We rewrite Eq. (5) using the expressions of the charging coefficients from Eqs. (A14)–(A16) to get a closed-form compact expression for steady state leakage current J_S . From the complete numerical simulations described in Appendix A, we observe that $A_{OUT} \gg A_{IN}$ in R₁ and $A_{IN} \gg A_{OUT}$ in R₂. We therefore neglect the terms that are small and write J_S as a sum of separate contributions from R₁ and R₂ (J_{S-R1} and J_{S-R2}). We thus derive the following expressions for J_{S-R1} and J_{S-R2} ,

$$J_{S-R1} = q\gamma N_T \exp\left(-\frac{\Phi_B - \beta\sqrt{E}}{k_B T}\right) \int_0^{x_1} \frac{\exp(\xi x) dx}{1 + \frac{q\gamma \exp(-\chi + \eta x)}{\alpha_{IN}}},$$

$$J_{S-R2} = q\gamma N_T \exp(-\chi) \int_{x_1}^{x_2} \frac{dx}{1 + \frac{q\gamma \exp(-\chi + \eta x)}{\alpha_{IN}}}$$

$$= q\gamma N_T \exp(-\chi) \left[x_2 - x_1 - \frac{1}{\eta} \log \left(\frac{q\gamma \exp(-\chi + \eta x_2) + \alpha_{IN}}{q\gamma \exp(-\chi + \eta x_1) + \alpha_{IN}} \right) \right]$$

$$= q\gamma N_T \exp(-\chi) \left[x_2 - x_1 - \frac{1}{\eta} \log \left(\frac{\frac{q\gamma}{\alpha_{IN}} \exp(-\chi) \exp(\eta x_2) + 1}{\frac{q\gamma}{\alpha_{IN}} \exp(-\chi) \exp(\eta x_1) + 1} \right) \right].$$

We find from simulations that, under high- E conditions and using typical values for the dielectric parameters, the denominator inside the logarithm term can be approximated by 1 and the numerator can be approximated by neglecting the 1. Therefore,

$$J_{S-R2} \approx q\gamma N_T \exp(-\chi) \times \left[x_2 - x_1 - \frac{1}{\eta} \log \left(\frac{q\gamma}{\alpha_{IN}} \exp(-\chi) \exp(\eta x_2) \right) \right],$$

$$J_{S-R2} = q\gamma N_T \exp(-\chi) \left[x_2 - x_1 - \frac{1}{\eta} \log \left(\frac{q\gamma}{\alpha_{IN}} \right) + \frac{\chi}{\eta} - x_2 \right],$$

$$J_{S-R2} = q\gamma N_T \exp(-\chi) \left[\frac{1}{\eta} \log \left(\frac{\alpha_{IN}}{q\gamma} \right) + \frac{\chi}{\eta} - x_1 \right].$$

Also, since J_S is a sum of J_{S-R1} and J_{S-R2} ,

$$J_S = J_{S-R1} + J_{S-R2}. \quad (\text{A18})$$

¹M. L. Green, E. P. Gusev, R. Degraeve, and E. L. Garfunkel, *J. Appl. Phys.* **90**, 2057 (2001).

²T. Tanaka, *IEEE Trans. Dielectr. Electr. Insul.* **12**, 914 (2005).

³J. J. Yao, *J. Micromech. Microeng.* **10**, R9 (2000).

⁴N. Setter, D. Damjanovic, L. Eng, G. Fox, S. Gevorgian, S. Hong, A. Kingon, H. Kohlstedt, N. Y. Park, G. B. Stephenson, I. Stolitchnov, A. K.

- Taganstev, D. V. Taylor, T. Yamada, and S. Streiffer, *J. Appl. Phys.* **100**, 051606 (2006).
- ⁵A. Shah, P. Torres, R. Tscharnner, N. Wyrsh, and H. Keppner, *Science* **285**, 692 (1999).
- ⁶P. D. Rack and P. H. Holloway, *Mater. Sci. Eng. R.* **21**, 171 (1998).
- ⁷D. L. Smith, *Thin-Film Deposition: Principles and Practice* (McGraw-Hill, New York, 1995).
- ⁸B. E. Deal and A. S. Grove, *J. Appl. Phys.* **36**, 3770 (1965).
- ⁹M. J. Powell, C. van Berkel, A. R. Franklin, S. C. Deane, and W. I. Milne, *Phys. Rev. B* **45**, 4160 (1992).
- ¹⁰J. Robertson and M. Powell, *Appl. Phys. Lett.* **44**, 415 (1984).
- ¹¹Y. Wang and T. Tseng, *J. Appl. Phys.* **81**, 6762 (1997).
- ¹²H. Wong and V. A. Gritsenko, *Microelectron. Reliab.* **42**, 597 (2002).
- ¹³W. M. van Spengen, R. Puers, R. Mertens, and I. De Wolf, in *International Electron Devices 2002 Meeting, Technical Digest* (IEEE, New York, 2002), pp. 901–904.
- ¹⁴E. G. Lee, D. J. Wouters, G. Willems, and H. E. M. Maes, *Appl. Phys. Lett.* **69**, 1223 (1996).
- ¹⁵C. Groves, J. C. Blakesley, and N. C. Greenham, *Nano Lett.* **10**, 1063 (2010).
- ¹⁶W. J. Tsai, S. H. Gu, N. K. Zous, C. C. Yeh, C. C. Liu, C. H. Chen, T. Wang, S. Pan, and C. Lu, in *40th Annual Reliability Physics Symposium Proceedings, 2002* (IEEE, New York, 2002), pp. 34–38.
- ¹⁷S. Melle, D. De Conto, L. Mazonq, D. Dubuc, K. Grenier, L. Bary, O. Vendier, J. L. Muraro, J. L. Cazaux, and R. Plana, in *2005 IEEE MTT-S International Microwave Symposium* (IEEE, New York, 2005), Vols. 1–4, pp. 757–760.
- ¹⁸T. P. Ma, *IEEE Trans. Electron Devices* **45**, 680 (1998).
- ¹⁹H. Hirose and Y. Wada, *Jpn. J. Appl. Phys.* **4**, 639 (1965).
- ²⁰J. Frenkel, *Phys. Rev.* **54**, 647 (1938).
- ²¹H. Kwon, I. Han, S. Park, J. Bok, Y. Jung, H. Shin, C. Kang, B. Lee, R. Jammy, G. Lee, and H. Lee, *Jpn. J. Appl. Phys.* **50**, 04DD02 (2011).
- ²²F. Engelman, J. Westlinder, G. F. Iriarte, I. V. Katardjiev, and J. Olsson, *IEEE Trans. Electron Devices* **50**, 1214 (2003).
- ²³C. H. Cheng, S. H. Lin, K. Y. Jhou, W. J. Chen, C. P. Chou, F. S. Yeh, J. Hu, M. Hwang, T. Arikado, S. P. McAlister, and A. Chin, *IEEE Electron Device Lett.* **29**, 845 (2008).
- ²⁴M. Thomas, J. Piquet, A. Farcy, C. Bermond, J. Torres, T. Lacrevez, B. Flechet, N. Casanova, C. Perrot, P. Caubet, and B. Chenevier, *Microelectron. Eng.* **82**, 521 (2005).
- ²⁵A. Jonscher, *Thin Solid Films* **1**, 213 (1967).
- ²⁶R. G. Southwick, J. Reed, C. Buu, R. Butler, G. Bersuker, and W. B. Knowlton, *IEEE Trans. Device Mater. Reliab.* **10**, 201 (2010).
- ²⁷J. Simmons, *Phys. Rev.* **166**, 912 (1968).
- ²⁸S. B. Bibyk and V. J. Kapoor, *J. Appl. Phys.* **52**, 7313 (1981).
- ²⁹G. Bersuker, J. Sim, C. S. Park, C. Young, S. Nadkarni, R. Choi, and B. H. Lee, *IEEE Trans. Device Mater. Reliab.* **7**, 138 (2007).
- ³⁰C. D. Young, Y. Zhao, D. Heh, R. Choi, B. H. Lee, and G. Bersuker, *IEEE Trans. Electron Devices* **56**, 1322 (2009).
- ³¹R. P. Johnson, D. W. Winslow, and C. C. Williams, *J. Appl. Phys.* **98**, 052902 (2011).
- ³²M. Masuduzzaman, A. E. Islam, and M. A. Alam, *IEEE Trans. Electron Devices* **55**, 3421 (2008).
- ³³D. Lang, *J. Appl. Phys.* **45**, 3023 (1974).
- ³⁴J. V. Li and D. H. Levi, *J. Appl. Phys.* **109**, 083701 (2011).
- ³⁵G. D. Wilk, R. M. Wallace, and J. M. Anthony, *J. Appl. Phys.* **89**, 5243 (2001).
- ³⁶M. Städele, B. R. Tuttle, and K. Hess, *J. Appl. Phys.* **89**, 348 (2001).
- ³⁷A. Gehring and S. Selberherr, *IEEE Trans. Device Mater. Reliab.* **4**, 306 (2004).
- ³⁸G. A. Dussel and K. W. Böer, *Phys. Status Solidi B* **39**, 375 (1970).
- ³⁹M. J. Kirton and M. J. Uren, *Appl. Phys. Lett.* **48**, 1270 (1986).
- ⁴⁰S. C. Miller and R. H. Good, *Phys. Rev.* **91**, 174 (1953).
- ⁴¹R. Hill, *Philos. Mag.* **23**, 59 (1971).
- ⁴²S. Manzini, *J. Appl. Phys.* **62**, 3278 (1987).
- ⁴³Y. Shusterman, N. Yakovlev, and L. Schowalter, *Appl. Surf. Sci.* **175–176**, 27 (2001).
- ⁴⁴Y.-P. Zhao, G.-C. Wang, T.-M. Lu, G. Palasantzas, and J. Th. M. De Hosson, *Phys. Rev. B* **60**, 9157 (1999).
- ⁴⁵P. C. Arnett, *J. Appl. Phys.* **46**, 5236 (1975).
- ⁴⁶T. A. Davis, *Direct Methods for Sparse Linear Systems* (SIAM, Philadelphia, PA, 2006).