Chapter 2
General Theories

Abstract In this section, we present a general survey of the theories and models that have been used to describe dielectric breakdown in amorphous thin films. The fundamental concepts for each theory are presented as initially proposed by the authors. Some of the models explained in this section include the $E, 1/E, \sqrt{E}$, power-law, and the metal-catalyzed failure model. Commentary on the limitations for each model is provided. In the latter part of this chapter, we will discuss the most recent models for describing reliability trends in contemporary interconnect structures that employ low-$\kappa$ nano-porous films. A general comparison between model predictions at low field is presented.

“Let others pride themselves about how many pages they have written; I’d rather boast about the ones I’ve read.”

—Jorge Luis Borges

2.1 Field Acceleration Models for Amorphous Thin Films

The study of gate oxide reliability established some of the most renowned time-dependent dielectric breakdown (TDDB) models. The $E$-model is one of the early attempts to extrapolate dielectric reliability from data at high-field and high-temperature conditions. The origin of the $E$-model can be traced to the late 1970s (Dumin 2002, p.135). This model is related to latent defect density, which is assumed to be randomly distributed in the dielectric matrix (Dumin 2002, p. 135–169; Anolick and Nelson 1980; McPherson and Mogul 1998). By definition, in the absence of stress, intrinsic defects do not contribute to dielectric failure. Upon application of an electric field, constraints in the dielectric lattice prevent relaxation of dipoles resulting in bond breakage at defect sites. Concurrently, as temperature increases, bonds in the dielectric matrix weaken, which facilitates dielectric degradation, resulting in failure.

Equation (2.1) shows the structure of the $E$-model. Here, $\Delta H_0$ is the enthalpy of activation, $T$ is temperature, $k_B$ is the Boltzmann constant, $\gamma$ is a field acceleration parameter, $A$ is a numerical constant, and TTF is time to failure (Fig. 2.1).
The $1/E$-model as originally postulated builds on the idea that failure is primarily a result of the accumulation of holes created by injected electrons through impact ionization across confined regions near the cathode. Electrons are injected from the cathode into the dielectric via Fowler–Nordheim tunneling (Chen et al. 1985a, b). Accumulation of these holes in confined regions increases the electric field near the cathode, which consequently causes electrons to tunnel, leading to a dramatic increase in localized current density (Chen et al. 1985a, b). The $1/E$-model has been predominant in TDDB studies primarily because the notion of dielectric degradation caused by charge transport is highly conceivable. The $1/E$-model was very effective at replicating TDDB data for high-field/high-current conditions. For low-field conditions, however, the $1/E$-model often deviated drastically from experimental results, and so a new correction was introduced, the hot-hole anode-injection model (Dumin 2002; Schuegraf and Hu 1994).

Schuegraf and Hu (1994) contemplated the idea that hot electrons might cause some damage to the dielectric matrix; however, only upon reaching the anode can hot electrons undergo full impact ionization. Hot holes are created by thermalization of the electrons with the dielectric lattice. Subsequently, these hot holes are able to tunnel into the dielectric and cause critical damage to the matrix. Equation (2.2) describes the $1/E$-model, where $G$ is the field acceleration parameter (Fig. 2.2).

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E\text{-Model : } \text{TTF} \propto A \cdot \exp\left(\frac{\Delta H_0}{K_B T}\right) \exp\left(-\gamma E\right).
$$

$$
1/E\text{-Model : } \text{TTF} \propto A \exp\left(\frac{\Delta H_0}{K_B T}\right) \exp\left(\frac{G}{E}\right).
$$

A very different dynamic from the $E$- and $1/E$-model is presented in the power-law model. This model was originally designed for thin-gate dielectrics. Here, it is said that carrier interaction with the matrix influences defect generation based on hydrogen release from the anode interface. Suñé and Wu (2004) attribute hydrogen release to electron-induced vibrational excitation of Si–H bonds. They argue that among the various proposed mechanisms for hydrogen release, coherent excitation is the most probable. Coherent excitation involves a single carrier exciting the bond to the highest energy state. At low energies ($<2.5$ eV), hydrogen release is primarily controlled by vibrational excitation, while electronic excitation becomes
predominant at high energies (above ~ 6.5 eV). For intermediate energies, both mechanisms participate in defect generation. Electronic excitation is generated by the incident carrier causing the transition of an electron from the bonding $\sigma$ state to the $\sigma^*$ antibonding state. The probability of defect generation ($\zeta$) by one injected electron is given in Eq. (2.2). Here, $A_{OX}$ is the oxide area, $B$ is the Weibull slope of the breakdown distribution, $q$ is the unit charge, $a_0$ is the linear size of defects, $T_{ox}$ is the oxide thickness, and $Q_{BD}$ is the charge to breakdown. According to Suñé and Wu (2004), time to failure scales with field in the same fashion as the probability of defect generation ($\zeta \propto E^{-m}$). The power-law model has been primarily employed in the study of failure for gate oxide and little- to low-κ interconnects. Wu and Suñé (2005) proposed a two-step defect generation process. Here carrier injection across the dielectric dissipates energy at the anode resulting in the release of holes and hydrogen species. These species can be transported into the dielectric matrix and further react with local defects to create a conducting path (Fig. 2.3).

$$\zeta = \frac{qT_{OX}}{a_0^2 Q_{BD}} \exp\left(-\frac{1}{B} \ln\left(\frac{A_{OX}}{a_0^2}\right)\right).$$  (2.3)

Power-law model: $\text{TTF} \propto t_0 E^{-m}$.  (2.4)

### 2.2 Emerging Models for Nano-porous Low-κ Films

The models presented in Sect. 2.1 describe various possibilities for how charge carriers participate in defect formation leading to dielectric breakdown. Such models have been applied for over 30 years to SiO$_2$ in predicting gate and interconnect reliability. However, for interconnects with low-κ spacing below...
90 nm, an additional mechanism for failure arises. For such systems, metal ions can migrate and accumulate in the dielectric matrix, assisting in the creation of percolation paths leading to catalyzed failure, which compromises the accuracy of conventional field acceleration models. This matter has been temporarily addressed by the use of diffusion barriers. However, as dielectric spacing between metal lines continues to scale down below 14 nm, such solutions will be challenged. In order to understand how ion injection affects failure, some authors have opted to develop TDDB models that include field acceleration parameters and energy barriers for ionic diffusion.

Recently Suzumura et al. (2006) and Chen et al. (2006) introduced a modified version of the $\sqrt{E}$-model initially proposed by Allers (2004) for intrinsic failure in Si$_3$N$_4$. Suzumura et al. (2006) state that electrons are transported across the dielectric via Poole–Frenkel tunneling. The migration of copper toward the cathode results in the lowering of barrier height for electron conduction. Ultimately, the accumulation of Cu ions changes the conduction mechanism to Fowler–Nordheim conduction. Dielectric failure occurs upon reaching a critical ion concentration near the cathode. Suzumura et al. (2006) found that failure dynamics agreed with the $\sqrt{E}$ behavior (Eq. 2.3). The $\beta_T$ parameter in Eq. (2.3) is equal to $\sqrt{q^3/4\pi\varepsilon\varepsilon_0}$, where $\varepsilon$ and $\varepsilon_0$ are the dielectric and vacuum permittivity, respectively.

Chen et al. (2006) modified the $\sqrt{E}$-model by including an expression for the critical concentration of ions due to the diffusion of Cu across the dielectric (Eq. 2.4). The $\sqrt{E}$-model as stated in Chen et al. (2006) is given in Eq. (2.5). Here, $A_R$ is equal to the effective Richardson constant, $D_0$ is the maximum diffusion coefficient, $t$ is the time, $l_0$ is total wire length, $\phi_s$ is the constant potential barrier, and $E_D$ is the activation energy for ionic diffusion. One of the disadvantages of Eq. (2.5) is that ion concentration across the dielectric matrix has been described using only ionic diffusion, which completely neglects the effects of ion drift by the
applied electric field and, more importantly, local field effects due to ionic charge, with the latter being significantly important for low-field extrapolation.

$$\sqrt{E} \text{-model: } \text{TTF} \propto A \exp \left( -2\beta T \sqrt{E} \right).$$ (2.5)

$$C_{\text{crit}} = 1.12 \cdot C_{\text{ions}} \sqrt{Dt},$$ (2.6)

Modified $\sqrt{E}$-model: $\text{TTF} \propto \frac{1}{T^4} \left( \frac{C_{\text{crit}} l_0}{D_0 A_R^2} \right) \exp \left( \frac{1}{k_B T} \left( E_D + 2\phi_S - 2\beta T \sqrt{E} \right) \right).$ (2.7)

Achanta et al. (2007, 2008) developed a more intuitive model to describe the contribution to dielectric failure of ionic injection. Here, ionic migration is described by a transient drift and diffusion model that takes into account local field contributions from ionic charge. Metal injection and electron transport simultaneously contribute to breakdown. Accordingly, Achanta et al. (2007, 2008) suggest that perhaps the contribution to degradation by ion transport could be integrated into an empirical field acceleration model to obtain a more accurate extrapolation expression. The $E^2$ correlation (Eq. 2.6) includes an exponential term that describes intrinsic bond breakage accelerated by the applied field and the ionic contribution (i.e., $f(C_{\text{ion}}, T, E_{\text{app}})$). The energy barrier associated to bond breakage is reduced by the applied field and is shown in Eq. (2.7). Here, $E_a^*$ is the effective activation energy for bond breakage under bias stress, $E_a$ is the intrinsic activation energy, $p$ is the permanent dipole moment for the dielectric matrix, $\alpha$ is the molecular polarizability, $E_{\text{loc}}$ is the local electric field, and $\gamma$ is the field acceleration parameter. The $E^2$ trend arises from the notion that at less than severe ionic migration into the dielectric matrix, the induced dipole moment energy term might dominate over the permanent dipole moment energy term. Thus, field dependence would be $E^2$. Achanta and McLaughlin (2011) expands the use of the metal injection $E^2$-model to breakdown in porous SiCOH. Here, a great correlation was found between model predictions and experimental data at low applied fields. Figure 2.4 illustrates the mechanism proposed by Achanta et al. (2008).

$$E^2 \text{-model: } \text{TTF} \propto A \exp \left( \frac{E_a^* - \gamma E_{\text{app}}^2}{k_B T} \right) f (C_{\text{ion}}, T, E_{\text{app}}),$$ (2.8)

$$E_a^* = E_a - p E_{\text{loc}} - \frac{1}{2} \alpha E_{\text{loc}}^2.$$ (2.9)

Hybrid models combining the $1/E$- and $\sqrt{E}$-model have been proposed in recent years (Lloyd et al. 2005, 2006). Lloyd et al. (2005) presents a model based on the idea that breakdown depends on the probability that electrons with enough energy can damage the dielectric when accelerated by an electric field. Lloyd et al. (2005) simply state that failure can be predicted without need to specify a failure mechanisms, because statistics of electron behavior ought to provide a quick
approximation for long-term reliability. The \((1/E + \sqrt{E})\)-model is shown in Eq. (2.8). Here, \(N_0\) and \(N_f\) represent initial and final defect concentrations and \(H\), \(\alpha\), and \(\gamma\) are constants. Lloyd et al. (2006) modified the \((1/E + \sqrt{E})\)-model to account for defect generation by the transport of metal ions. The analytical expression for the metal-catalyzed failure model is given in Eq. (2.9). \(N_0\) and \(N_f\) are the initial and final defect concentrations, \(D\) is the diffusion coefficient for Cu ions, \(z\) is the charge of Cu ions, \(V\) is the local potential, \(l\) is the effective dielectric thickness, and \(A\) and \(\alpha\) are empirical parameters.

\[
(1/E + \sqrt{E})\)-model: \quad \text{TTF} \propto \left(\frac{H}{E}\right) \exp\left(-\gamma\sqrt{E} + \frac{\alpha}{E}\right). \tag{2.10}
\]

Lloyd et al. (2006): \quad \text{TTF} \propto \left(\frac{k_B T}{D z e V}\right) \left( l^2 - \left[ \frac{V}{\alpha} \ln \left( \frac{(N_f - N_0) e D z e}{2 A V k_B T} + \exp \left(\frac{-a l}{V}\right) \right) \right] \right)^2. \tag{2.11}

The development of empirical models to describe the complex physical processes resulting in dielectric failure has recently been challenged by Haase (2009), who provided a paradigm shift in dielectric breakdown research for amorphous thin films. He proposed a model using nonlinear partial differential equations that describe the injection and conduction of charge carrier across the dielectric film. These equations provide a physical view of how electronic conduction can lead to defect formation and fatal distortions of the local electric field at the cathode. The latter is considered to be responsible for dielectric breakdown.

Nonetheless, there are major disadvantages to the theory presented by Haase (2009). It fails to include the transport of ionic species and fails to replicate the large

Fig. 2.4  Cu diffusion and drift due to applied electric field. Transport of Cu species into the dielectric assists on the formation of a conductive path. Figure based on Achanta et al. (2008)
instability in electronic conduction observed at failure. Figure 2.5 illustrates the mechanism proposed by Haase (2009).

Extrapolation of failure to low-field and low-temperature conditions remains a highly controversial subject. Authors fiercely defend their models and argue that experimental data support their empirical fits. Figure 2.6 describes such conflicting results and establishes the notion that perhaps TDDB for interconnect structures must be studied differently and that models ought to provide a mathematical description of the dynamics that generate dielectric failure rather than senseless empirical fits. In addition, all the models presented in the literature apply only to constant field conditions, which raises questions about their robustness for

Fig. 2.5 Carrier transport resulting in defect formation across the dielectric matrix. Defects accumulate to form a conductive path

Fig. 2.6 Time to breakdown vs. applied field, correlation between conventional dielectric and degradation models. (a) Correlation between TTF and literature models for Cu–SiCOH ($\kappa = 2.4$) inter-level structure, Achanta and McLaughlin (2014). (b) Correlation for Cu–SiO$_2$ MIS capacitor, Zhao et al. (2011). Courtesy of Achanta and McLaughlin (2014) and Zhao et al. (2011)
describing actual breakdown phenomena. The ideal extrapolation method is one that describes and predicts dielectric failure. Such a scheme might be achieved by integrating metal drift and electron transport into a single charge transport model.

Predictions shown in Fig. 2.6 range from the most conservative $E^2$-model all the way to the most optimistic $1/E$-model. Predictions at high field are for the most part matched by all models with high accuracy. However, at low field there is a serious deviation from model predictions as well as experimental data. Chery et al. (2013) presented low-field data collected for over 1 year (Fig. 2.7). Here, the author argues that experimental trends are best replicated by the $(1/E + \sqrt{E})$-model, also known as the lucky-electron (LE) model. If a conclusion can be drawn for the present section, it would be that no clear progress has taken place to resolve the long-term behavior of dielectric failure from data collected at high-field and high-temperature conditions. There is an obvious need to understand the innate features of the physical failure mechanism. Empirical fits and statistical expressions might not be the adequate direction.

References


Dielectric Breakdown in Gigascale Electronics
Time Dependent Failure Mechanisms
Borja, J.P.; Lu, T.-M.; Plawsky, J.
2016, VIII, 105 p. 74 illus., 33 illus. in color., Softcover
ISBN: 978-3-319-43218-2