

A TIME DEPENDENT DIELECTRIC BREAKDOWN (TDDB) MODEL FOR FIELD ACCELERATED LOW-K BREAKDOWN DUE TO COPPER IONS

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ABSTRACT

We have simulated the copper ion concentration and internal electric field profiles in a dielectric material by solving the transient continuity/Poisson equations. We have shown that failure of dielectrics can be modeled if we assume that failure in Cu/SiO₂/Si devices occurs due to a pile-up of copper ions at the cathode and the subsequent increase in electric field that accompanies the pile up. A comparison with experimental data shows that polarization of the dielectric due to the high field surrounding the copper ions contributes to acceleration of the breakdown and that breakdown in porous dielectrics is faster than solid dielectrics due to field concentration around the pores of the dielectric.

Keywords: Dielectric breakdown, low-k materials, copper injection

1. INTRODUCTION

Metal ion contamination of a dielectric material, resulting from long-term device operation or short term reliability testing under conditions of high temperature and high applied field, has been shown to lead to reliability problems and accelerated breakdown times [1 - 6].

The physical-chemical interactions of copper with the dielectric which lead to accelerated dielectric breakdown are not well understood. It is suggested that copper forms temporary energy levels, called traps in the bulk of the dielectric as it transits from the anode to the cathode [1 - 3]. Copper ions accumulate at the cathode, altering the local electric field, leading to Fowler-Nordheim tunneling of electrons across the interface. As these emitted electrons transit through the dielectric, accelerated by the applied field, they damage the structure of the dielectric leading to failure [3,6]. Thus dielectric breakdown may occur as a consequence of the electrons that are emitted as copper ions drift through the dielectric and pile up at the cathode.

A number of models have appeared in the literature to describe the time-dependent breakdown of low-k dielectrics. Lloyd et al. [4] briefly described these models and compared the time-to-failure of the dielectric based on the predictions of each model. In Lloyd et al's impact damage model, highly energetic electrons accelerated by the field damage the dielectric through impact ionization. The microscopic mechanisms which cause the damage are not specified and are considered unimportant. Breakdown occurs once a critical defect concentration is reached. The effect of copper ions in enhancing breakdown is approximated by reducing the spacing

between the anode and the cathode thus effectively raising the field in their model equations.

Chen et al.[2] considered that dielectric breakdown occurs once a critical copper concentration is reached. The copper ion leakage current was assumed to be Schottky in origin. In their model only molecular diffusion of copper ions was considered and drift was neglected. The $\ln(\text{time-to-failure})$ thus derived is shown to have a \sqrt{E} dependence.

Suzumura et al.[3] similarly considered that low-k breakdown occurs once a critical copper concentration accumulates inside the dielectric. The copper ion leakage current was shown to have a better fit to a Poole-Frenkel type mechanism than a Schottky mechanism. The final expression for $\ln(\text{time-to-failure})$ also has a \sqrt{E} dependence though Suzumura et al., unlike Chen et al., do not consider the effect of copper ion diffusion.

Haase et al. [7] applied the thermo-chemical E-model [8] to describe the breakdown in low-k dielectrics. In the thermo-chemical E-model, used extensively to predict time dependent dielectric breakdown (TDDB) for gate oxides, dielectric breakdown is believed to be caused due to bond breakage. The electric field reduces the activation energy for bond breakage accelerating breakdown. The field acceleration parameter (γ), which is determined experimentally, takes this effect into account. The time-to-failure (TTF) at low-fields is extrapolated from the γ obtained at high fields. The effect of copper ions is not considered explicitly.

In all the models considered above the exact value of the critical defect density or the critical copper concentration necessary to cause breakdown is unknown. The dependence of copper transport and copper solubility, and interfacial boundary conditions is also not addressed. In this paper, we extend the E-model to explicitly include the effect of mass transport of copper ions on the time-to-failure while at the same time showing the implications of copper ion solubility and interfacial boundary conditions on the time to failure.

2.0 MODEL DEVELOPMENT

We have modeled the mass transport of copper ions in one and two dimensions using the geometries in Figure 1 and solved the combined non-linear continuity and Poisson equations to obtain the concentration and electric field profiles in the dielectric [9]. We showed that the choice of boundary conditions at the cathode is critical and that the blocking electrode condition ($J(t,L)=0$) is the physically correct one to use [9]. The use of this

boundary condition leads to an accumulation of copper ions at the cathode increasing the internal electric field there. SIMS analysis of copper contaminated interconnect dielectrics has shown that copper ions do accumulate at the cathode interface suggesting that this is the correct boundary condition [10 - 12]. We showed that time to failure could be correlated with the time required for the field at the cathode to reach the intrinsic breakdown strength of the dielectric. A similar explanation was used for analyzing gate dielectric breakdown in thermal oxides due to sodium contamination [13 - 15]. It was suggested that the enhanced failure rates occurred due to an increase in the internal field as sodium ions accumulated at the cathode [16,17]. Thus, the failure criterion for copper contaminated interconnect dielectrics and sodium contaminated gate dielectrics appear to be similar.

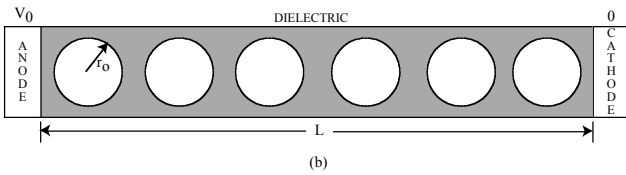
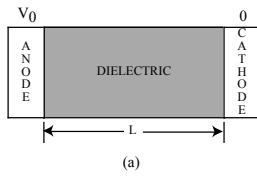


Figure 1 Model geometries for time-to-failure simulations. The upper figure is for a solid dielectric, the lower for a porous dielectric.

The model for field assisted copper migration through the dielectric is given by:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} + \mu \frac{\partial}{\partial x} \left(C \frac{\partial V}{\partial x} \right) \quad \text{Continuity Equation} \quad (1)$$

$$J(t, x) = -D \frac{\partial C}{\partial x} - \mu C \frac{\partial V}{\partial x} \quad \text{Flux} \quad (2)$$

The system of equations is made dimensionless using the following scaling relations.

$$\chi = \frac{C}{C_e} \quad v = \frac{V}{V_e} \quad \xi = \frac{x}{L} \quad \tau = \frac{tD}{L^2} \quad (3)$$

The Einstein relation gives ties the ion mobility to its diffusivity through the thermal voltage, V_e ,

$$\frac{D}{\mu} = V_e \quad V_e = \frac{k_B T}{q} \quad (4)$$

and so equation (1) becomes:

$$\frac{\partial \chi}{\partial \tau} = \frac{\partial^2 \chi}{\partial \xi^2} + \frac{\partial}{\partial \xi} \left(\chi \frac{\partial v}{\partial \xi} \right) \quad (5)$$

Equations (1) and (2) are coupled to one another via a dimensionless form of Poisson's equation:

$$\frac{\partial^2 v}{\partial \xi^2} = - \left(\frac{q C_e L^2}{k_D \epsilon_0 V_e} \right) \chi = -Q \chi \quad (6)$$

The initial and boundary conditions are:

$$\chi(0, \xi) = 0 \quad v(0, \xi) = 0 \quad (7)$$

$$\chi(\tau, 0) = 0 \quad v(\tau, 0) = \frac{V_0}{V_e} \quad (8)$$

$$\left. \frac{\partial \chi}{\partial \xi} \right|_{\xi=1} + \chi \left. \frac{\partial v}{\partial \xi} \right|_{\xi=1} = 0 \quad v(\tau, 1) = 0$$

where C_e is metal solubility in the low-k dielectric at the conditions of the test. Note that in dimensionless form, this system of equations is fixed once V_0/V_e and Q are specified.

We calculated the time, $f(C_e, T, E_{app})$ that it takes for the internal electric field at the cathode to increase to the breakdown strength of the dielectric ($E_{bd}=10$ MV/cm) at any particular temperature and electric field using the equations described above. This time $f(C_e, T, E_{app})$ is a function of C_e , the solubility of copper in the dielectric (assumed to be a constant whose range is between $3 \times 10^{17} - 3 \times 10^{19}$ at/cm³ for thermal SiO₂ [18 - 20]). The time also depends on the applied electric field and the temperature T . The diffusivity depends on the temperature and was assumed to be concentration independent. We used with $D_0 = 1.68 \times 10^{-10}$ cm²/s, $E_a = 0.653$ eV [21].

Mass transfer alone cannot completely describe time to failure. Dielectric failure occurs even in the absence of copper ions and is believed to be due to thermally activated bond breakage. The applied field reduces the activation energy for bond breakage as shown in equation (9) [8].

$$E_a^* = E_a - pE_{loc} - \frac{1}{2} \alpha E_{loc}^2 \quad (9)$$

In the presence of copper ions, the induced dipole moment energy ($\frac{1}{2} \alpha E_{loc}^2$) of amorphous SiO₂ is greater than the permanent dipole energy (pE_{loc}) and lead us to formulate an expression for time to failure by combining the effects of mass transfer and intrinsic thermochemical bond breakage effects [22,23]. The time to failure (TTF) is represented by an expression of the form:

$$TTF(s) = A \exp\left(\frac{E_a - \gamma E_{app}^2}{k_B T}\right) f(C_e, T, E_{app}) \quad (10)$$

3.0 RESULTS

We have shown in Figure 2 that the equation fits the TTF experimental data for Cu/SiO₂/Si capacitors over a broad range of temperatures (150°C -250°C) and applied fields (1-4 MV/cm) using single values of A(2x10⁻¹³), γ (.015) and E_a(1.15 eV) [22]. The model also successfully simulates the non-linearity in the TTF curve at low applied fields as was experimentally observed [22].

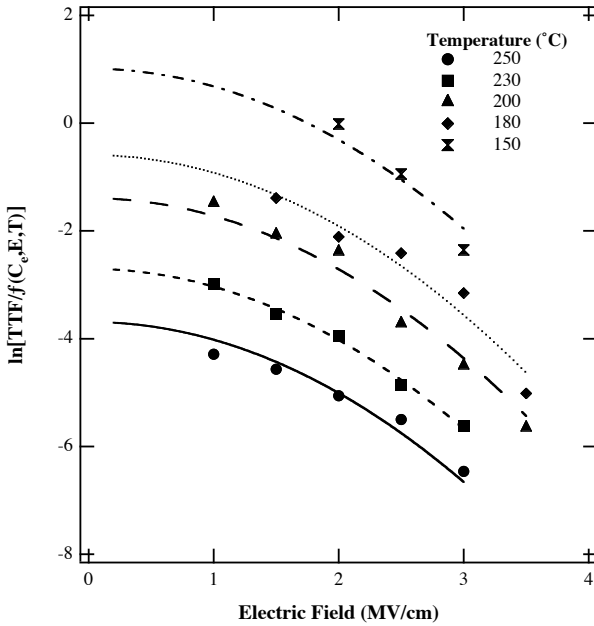


Figure 2 Fit of experimental time to failure data using equation (10). Curvature indicates that a linear dependence on the applied electric field is incorrect.

Though the model was successful in predicting the time-to-failure in SiO₂ the predicted values for the concentration of copper ions at the cathode at the point where breakdown occurs were large. Though the reported solubility of Cu in SiO₂, C_e, varies by nearly two orders of magnitude (3x10²³ – 3x10²⁵ atoms/m³), the predicted values were still higher. This indicated that some mass transfer mechanism must be missing from the model.

Previous investigators working on sodium ion drift in thermal SiO₂, included an additional flux term to account for the interaction of the ion with the dielectric medium [24]. This term, which amounts to a concentration dependent diffusion coefficient, was included to simulate the dielectric's resistance to being stuffed with high concentrations of ions. It is akin to a coefficient of volume expansion. Similar resistances were reportedly observed in work on impurity diffusion in solids [25,26]. The additional flux termed an elastic drift, is given by:

$$J_{elastic} = -\left(\frac{\alpha D}{k_B T}\right) C \frac{\partial C}{\partial x} \quad (11)$$

α is the elastic energy coefficient and relates the energy of ion interaction with the medium. A value of α = 2 x 10⁻⁴⁴ Jm³ for thermal SiO₂ has been reported. With the inclusion of this new term the continuity equation becomes:

$$\frac{\partial \chi}{\partial \tau} = \frac{\partial}{\partial \xi} \left\{ \frac{\partial \chi}{\partial \xi} \left[1 + \left(\frac{\alpha}{k_B T} \right) \chi \right] \right\} + \frac{\partial}{\partial \xi} \left(\chi \frac{\partial v}{\partial \xi} \right) \quad (12)$$

while the Poisson equation remains unchanged.

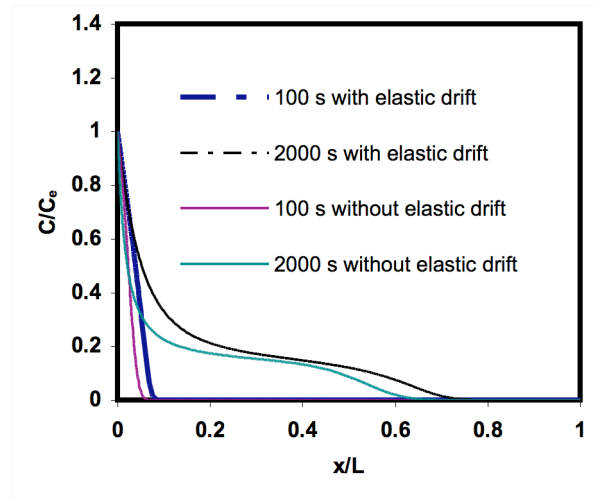


Figure 3 Cu concentration profiles in the dielectric with and without the extra elastic drift term.

As shown in Figure 3 the inclusion of the additional term in equation (12) slightly increases the depth of Cu penetration into the bulk of the dielectric and if the time to failure were based solely on a breakthrough of Cu ions, this term would decrease the time to failure. However at the cathode, the additional term serves to decrease the concentration and concentration gradient there. We plot C(L)/C_e as a function of E_{app} at 250°C with and without the elastic drift term. As can be seen in Figure 4, the value of C(L)/C_e is nearly two orders of magnitude lower with the inclusion of the elastic drift term. The new value of C(L)/C_e seems to be more reasonable and if we use C_e at the upper limit of the experimentally reported value, we simulate breakdown once C(L) reaches C_e, a physically more realistic situation. Though the C(L)/C_e ratio drops dramatically, there is very little change in the time required for E(L) to reach E_{bd}, as seen in Figure 5, in the applied field range (1 MV/cm-3.5 MV/cm). Thus, aside from changing the value of C(L) at failure, the inclusion of the elastic drift term does not alter our earlier predictions for the time to failure in the higher electric field range (1 MV/cm-3.5 MV/cm). At low electric fields, when the drift component of mass transfer is smaller, there seems to be a difference with and without elastic drift term. Inclusion of the elastic drift term shows that there is a maximum applied field below which failure will

never occur. This maximum field is nominally higher than the fields under which devices normally operate. The prediction of this model must still be evaluated experimentally. The problem is that the time required to run the experiments is very long and could be much longer than the normal time required to update and introduce new microprocessors.

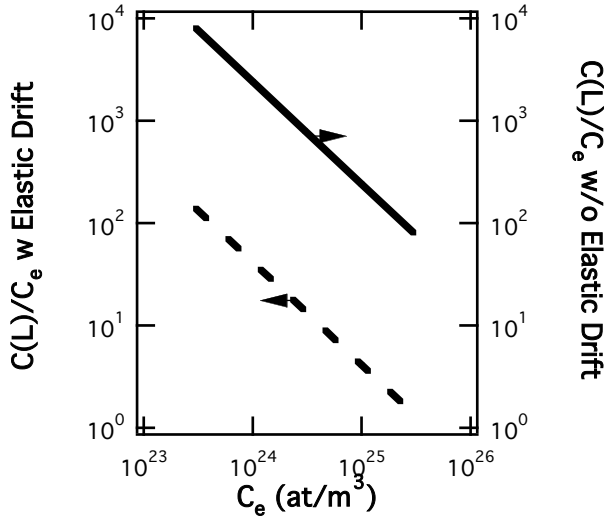


Figure 4 Cu concentration at the cathode when breakdown occurs. The temperature associated with the simulation is 250 °C. Breakdown occurs at the solubility limit if $C_e = 4.2 \times 10^{25}$ atoms/m³, close to the maximum reported literature value.

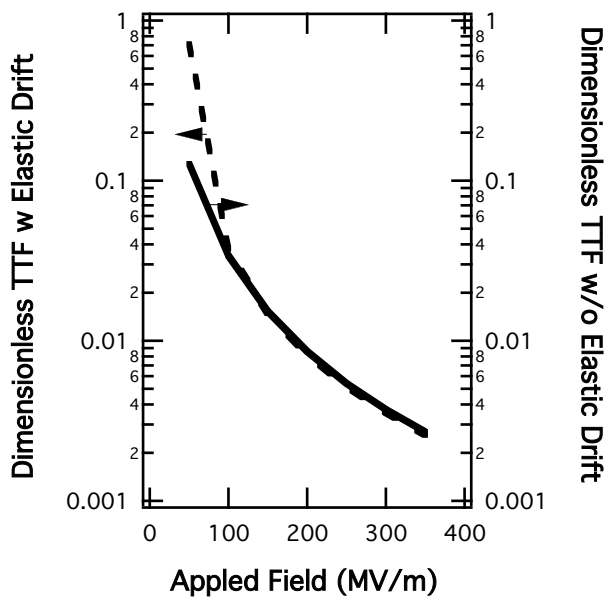


Figure 5 Dimensionless time-to-failure with and without the elastic drift component. Time-to-failure is similar for applied fields in excess of 100 MV/m. Simulation conducted for $C_e = 3 \times 10^{24}$ atoms/m³ and $T = 250$ °C.

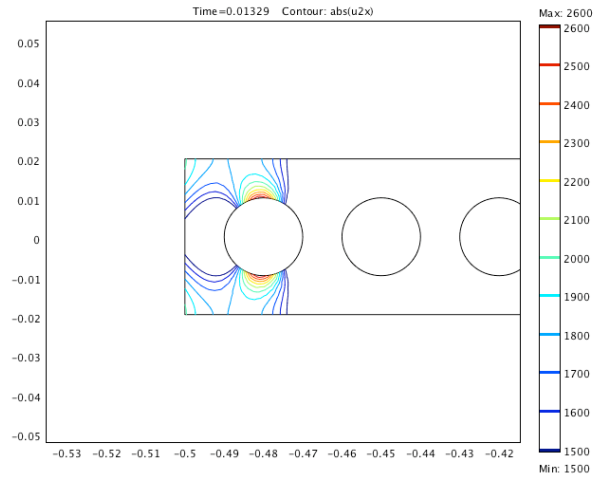


Figure 6 Electric field strength in a region near the anode of the dielectric stack.

Newer generations of microprocessors will be built with porous, low-k dielectric materials. Experimental data suggests that these materials fail much faster than dense versions of the same material. To attempt to understand this behavior, 2-D versions of the simulation were conducted using the geometry in Figure 1. Figures 6 and 7 show the results of these simulations and present contour plots of the electric field strength near the anode and cathode respectively. The dielectric was assumed to be 100 nm thick with 2 nm pores and have an overall porosity of 50%. In this case the simulation was performed at 250 °C, with $C_e = 3 \times 10^{24}$ atoms/m³ and at an applied field of 100 MV/m. The results indicated that failure occurred faster for the porous version and the reason for the failure was the concentration of the field in the region near the pores. As the field lines show, the field is concentrated at the equivalent of the separation point for laminar flow about a sphere. This kind of solu-

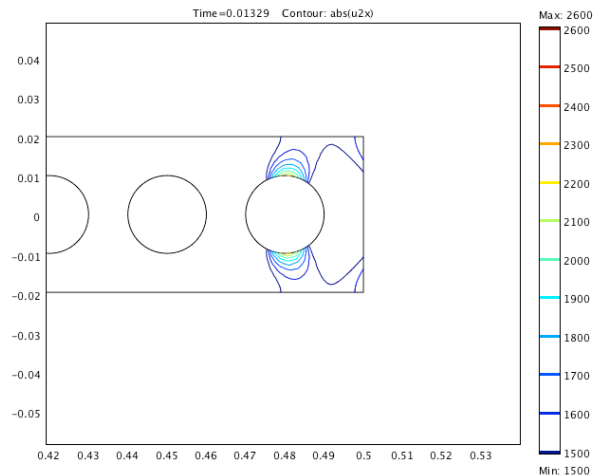


Figure 7 Electric field strength in a region near the cathode of the dielectric stack.

tion agrees with experimental observations which indicate that final failure occurs at a point and that failure requires mirror conditions at both anode and cathode

ends. It is still unclear whether final failure occurs due to hole injection from the anode or electron injection from the cathode.

5.0 CONCLUSIONS

Failure of a dielectric in the presence of injected Cu ions was simulated by solving transient versions of the continuity and Poisson equations with and without an elastic drift term. The model indicates that it is the induced polarization of the dielectric that is responsible for the decrease in the time to failure once metal ions are presented. The inclusion of the elastic drift term resolves the issue of unreasonably high values of copper ions at the cathode at the time of failure and allows failure to occur once the concentration of Cu ions saturates at the cathode. Two-dimensional simulations of porous materials show that failure occurs faster than for comparable dense dielectrics and that such failure is accelerated due to concentration of the electric field at the pores of the dielectric.

6.0 ACKNOWLEDGEMENTS

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7.0 REFERENCES

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