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Reliability Testing for the Next Generation of Microelectronic Devices

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ABSTRACT

Reliability testing of microelectronics devices involves operation at high temperatures and high applied fields as a means of accelerating failure and obtaining results in a reasonable amount of time. We are concerned primarily with describing the effects of copper ion injection on dielectric breakdown. Experimentally, these effects are characterized though current-time (I-t) and current-voltage (I-V) testing. Using our mass transport-based failure description coupled with Comsol simulations, we have been able to relate the two failure test procedures and develop alternative versions of those testing procedures that yield more useful information than the standard methods. The theoretical predictions we made are confirmed by experiment and can be show to arise naturally through a simple change in the boundary conditions of our Comsol model.

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

1. INTRODUCTION

Dielectric breakdown can occur via a number of mechanisms depending on whether the dielectric is exposed to high temperatures, high electric fields, or both conditions simultaneously. 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 accelerated breakdown times [1 - 6]. The metals can be assumed to catalyze the breakdown.

The processes leading to dielectric breakdown are still not well understood. It widely thought that hot electrons and holes transit through the dielectric, become accelerated by the applied field and damage the structure of the dielectric leading to failure [3,6]. It has also been 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 enhanced rates of Fowler-Nordheim tunneling of electrons across the interface. Thus dielectric breakdown is enhanced 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 that cause the damage were not specified. Breakdown was assumed to occur once a critical defect concentration was reached. The effect of copper ions in enhancing breakdown was approximated by reducing the spacing between the anode and the cathode thus effectively raising the applied 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 *In*(time-to-

failure) thus derived was 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 *In*(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 Emodel [8] to describe the breakdown in low-k The E-model assumes dielectric dielectrics. breakdown is caused by 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. Haase [9] later developed a trap generation model that tied the hot electron flux into the dielectric to trap creation and subsequently breakdown. The results of this mode were consistent

with the E-model lending credibility to the use of the E-model as simple, but accurate tool.

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. Thus one cannot predict a priori when a dielectric will break down given a value of the applied field and temperature, or at what applied field a dielectric will break down given an operating temperature. More sophisticated experiments and models are necessary.

2.0 MODEL DEVELOPMENT

We have modeled the mass transport of copper ions using the geometry and conceptual process shown in Figure 1 [10-12]. The mechanism for copper's contribution to failure involves the oxidation of copper metal at the metal-dielectric interface. The metal ions generated by the oxidation then are injected into the dielectric. The ions are driven by the electric field toward the dielectric-Si interface where they accumulate. Eventually, the local electric field rises to a critical value we term the intrinsic breakdown field, and at that point, the field is high enough to promote easy tunneling of electrons across the barrier leading to breakdown.

We have solved the combined non-linear continuity and Poisson equations to obtain the Cu concentration and electric field profiles in the dielectric [10-12]. We have shown that the model can reproduce experimental data for SiO_2 dielectrics, SiCOH dielectrics, and systems that include a diffusion barrier between the metal and the dielectric

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

Continuity Equation

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

Cu Ion Flux

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

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

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

The Einstein relation gives ties the ion mobility to its diffusivity through the thermal voltage, V_{e} ,



Figure 1 Model schematic for time-to-failure simulations. Catastrophic failure is assumed to occur once the copper ion accumulation at the Si-Dielectric interface is high enough to promote massive injection of electrons into the dielectric..

$$\frac{D}{\mu} = V_e \qquad \qquad V_e = \frac{k_B T}{q} \tag{4}$$

and so equation (1) becomes:

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

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

$$\frac{\partial^2 \upsilon}{\partial \xi^2} = -\left(\frac{qC_e L^2}{k_D \varepsilon_0 V_e}\right) \chi = -Q\chi \tag{6}$$

The initial and boundary conditions are:

$$\chi(0,\xi) = 0$$
 $\upsilon(0,\xi) = 0$ (7)

$$\chi(\tau,0) = 0 \qquad \qquad \upsilon(\tau,0) = \frac{V_0}{V_e}$$

$$\left. \frac{\partial \chi}{\partial \xi} \right|_{\xi=1} + \chi \left. \frac{\partial \upsilon}{\partial \xi} \right|_{\xi=1} = 0 \qquad \upsilon(\tau,1) = 0$$
(8)

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 V₀/V_e and Q are specified.

3.0 RESULTS

There are two primary testing procedures used to evaluate breakdown, current-time testing, and current-voltage testing. Both are shown in Figure 2. Current-time tests operate by applying a steady electric field to a device at elevated temperature. Failure is assumed once the current passes a threshold value and the process defines a time-tofailure. Current-voltage testing operates by applying a continuously increasing voltage to a device under elevated temperature. Failure is assumed to occur once the current passes a threshold and the process defines a breakdown field for the dielectric.

Though current-time tests more accurately simulate the wear-out and breakdown of dielectrics, current-voltage testing is more common since the voltage can be ramped fairly quickly and so the tests take little time. If the scenario shown in Figure 1 holds, then a current-voltage test should be affected by metal ion drift if the test were conducted over a sufficiently long time span. The test should also be able to distinguish between reactive metal anodes such as copper and inert metal anodes such as gold or aluminum.

We decided to test this hypothesis by running current-voltage tests and varying the voltage ramp rate over several orders of magnitude. Since metal ion diffusion and drift are slow, timescales on the order of hundreds of minutes are required. Our scenario predicted that for inert metal anodes, the breakdown voltage or breakdown field determined using a current-voltage test should be independent of the voltage ramp rate. If the anode were made of a reactive metal, the breakdown field should be highly dependent on the voltage ramp rate.



Figure 2 Typical results from an (a) I-t and an (b) I-V test. Dielectric breakdown was assumed to occur when the current exceeded 10^{-5} amps.

Figure 3 shows the result of a number of currentvoltage tests on a SiCOH-based dielectric using aluminum and copper metallization. The tests were conducted at 250 °C. In these tests the applied voltage was increased using a linear ramp rate ranging from 0.001 V/s up to a maximum of about 10 V/s. The results show a clear difference in behavior between the aluminum and copper metallization. The breakdown behavior for aluminum metallization is independent of voltage ramp rate over a very large range, especially at the lower ramp rates where one would expect the effects of metal ion drift to be prominent. Since aluminum must exist in silicabased materials in a +3 ionic state, very little, if any of it, can enter into the dielectric under the conditions of the test. There are no regions within the dielectric that can accommodate an ion of such high charge. At the highest ramp rates we see another abrupt jump in breakdown voltage for the aluminum. We believe this jump is an artifact of our equipment. The

(9)

equipment cannot measure the current accurately at those high voltage ramp rates.

The copper metallization results are highly dependent upon the ramp rate. The dielectric breakdown strength decreases with decreasing ramp rate. This result is consistent with the scenario shown in Figure 1 since at the lower ramp rates, copper penetration and accumulation at the cathode has time to occur. The accumulation increases the local electric field at the cathode (Si) end and allows for electrons to tunnel into the dielectric. Copper can enter the dielectric readily since it can exist in silicabased materials either in a +1 or +2 ionic state.



Figure 3 Current-voltage tests results for a SiCOH dielectric using either aluminum or copper anodes. The applied voltage was increased using a linear ramp rate at the values specified in the figure.

The experiment provides more useful information. If the aluminum acts as an inert anode material, then the breakdown field strength we measure is due solely to electron and hole bombardment. The value of the breakdown field extrapolated to an infinitesimal voltage ramp rate would then be what we call the intrinsic breakdown strength; a key parameter needed in the transport models we have developed. There is likely a lower limit for the breakdown strength using copper as the anode material. We refer to this as the minimum copper concentration required for breakdown and represents the critical concentration of copper below which insufficient copper exists to drive the local electric field at the cathode to exceed the intrinsic breakdown strength of the dielectric as determined by the aluminum anode results.

Both I-t and I-V testing can be simulated using our transport-based model. The model provides a way of linking and relating the two tests. In either test case, the requirement for breakdown was the same; exceeding a given current threshold. In our transport model, we translate that condition into requiring the local electric field at the cathode to exceed the intrinsic breakdown strength of the dielectric. Thus, in Comsol, we continuously monitor the local electric field at the cathode boundary and stop the solution using a stop condition once that field reaches our predefined threshold. To simulate the process of an I-V test, all that is required is to change the boundary condition at the anode. During the I-V test, the voltage is of the form V(t) = a*t + b. Thus equation (8) becomes:

$$\chi(\tau,0) = 0 \qquad \qquad \upsilon(\tau,0) = \frac{V_0(t)}{V_e} = \frac{at+b}{V_e}$$

$$\frac{\partial \chi}{\partial \xi}\Big|_{\xi=1} + \chi \frac{\partial \upsilon}{\partial \xi}\Big|_{\xi=1} = 0 \qquad \upsilon(\tau, 1) = 0$$

and a simple change in the boundary condition at the anode is all that is needed to switch the model from simulating an I-t test to simulating an I-V test.

The key piece of information needed to stop the model is the intrinsic breakdown strength of the dielectric. Using the information from the aluminum tests shown in Figure 3, we estimated the breakdown strength of the dielectric to be 4.5 MV/cm. Thus the simulation would end once the local electric field at the cathode exceeded 4.5 MV/cm.

Figure 4 shows the results of the simulation compared with the experimental data for copper replotted from Figure 3. The simulation was performed for a SiCOH-based material that was 200 nm thick, had a dielectric constant of about 3, and was being tested at 250 °C. The simulation is able to reproduce the trends we see in the experiment and the fit of the simulation results to the experimental results is surprisingly good. We say this because key parameters used in the model such as the diffusivity of copper ions in the dielectric and the solubility of copper ions in the dielectric are unknown for SiCOHbased materials. We simply used the best values for those parameters that we could obtain for SiO₂. Since SiCOH materials have much more organic character and are much more hydrophobic than SiO₂. there is no real reason to believe that either the solubility or diffusivity is the same in both materials. The only piece of experimental data we have for SiCOH is the value of the intrinsic breakdown field strength and though we used that value based on the aluminum experiments, we have some evidence that the intrinsic breakdown field for a copper anode may be a bit different than 4.5 MV/cm due to the difference in electron affinity between copper and aluminum. More experimental work coupled with Comsol simulations should help us resolve these issues and achieve better agreement between the experiment and the simulation.



Figure 4 Applied electric field at the onset of breakdown. Symbols represent the experimental data using a copper anode. The solid line shows a premliminary fit of the data using Comsol simulation of the process

4.0 CONCLUSIONS

Failure of a dielectric in the presence of injected Cu ions was simulated by solving the transient versions of the continuity and Poisson equations using Comsol. The transport model developed in Comsol was instrumental in helping us understand how to tie the two major failure testing procedures, I-t and I-V testing, together. We showed that a simple change to the boundary condition at the anode would allow us to transform the model from one that was simulating an I-t test to one that was simulating an I-V test. Experimentally, we showed that running an I-V test using a variable voltage ramp rate provided more information about how a dielectric may fail than running a single ramp rate test. Simulations using Comsol were able to reproduce the experimental trends and even match the data to a reasonable extent given the uncertainly in the material parameters used in the model.

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6.0 NOMENCLATURE

С	copper ion concentration in the dielectric	q	electron charge
C _e	copper solubility in the dielectric	Т	temperature
D	copper ion diffusivity in the dielectric	V	voltage
Eann	applied electric field	Ve	thermal voltage
J	flux of cu in the dielectric	Vo	applied voltage
k _B	Boltzmann's constant	ε	permittivity of a vacuum
k _D	dielectric constant	μ	mobility of copper ions
L	dielectric thickness		

7.0 REFERENCES

- 1) Chen, F. et al., (2005) in *Proceedings of the International Reliability Physics Symposium* (IEEE, New York, 2005), p501.
- Chen, F., Bravo, O., Chanda, K., McLaughlin, P., Sullivan, T., Gill, J., Lloyd, J., Kontra, R., and Aitken, J., (2006) in *Proceedings of the International Reliability Physics Symposium* (IEEE, New York, 2006), p46.
- Suzumura, N., Yamamoto, S., Kodama, D., Makabe, K., Komori, J., Murakami, E., Maegawa, S., and Kubota, K., (2006) in Proceedings of the International Reliability Physics Symposium (IEEE, New York, 2006), p 484.
- Lloyd, J.R., Murray, C.E., Ponoth, S., Cohen, S., and Liniger, E.G., *Microlectronics Reliability*, 46, 1643.
- 5) Gonella, R., (2001) Microlectron. Engg., 55, 245.
- 6) Loke, A.L.S., Wetzel, J.T., Townsend, P.H., Tanabe, T., Vrtis, R.N., Zussman, M.P., Kumar, D.K., Ryu, C., and Wong, S.S., (1999) *IEEE Trans. Electron Devices* **46**, 2178.
- Haase, G.S., Ogawa, E.T., and McPherson, J.W., (2005) in *Proceedings of the International Reliability Physics Symposium* (IEEE, New York, 2005), p 466.
- 8) McPherson, J.W. and Mogul, H.C., (1998) *J.Appl.Phys.*, **84**, 1513.
- Haase, G.S., J. Appl. Phys., 105, 044908 (2009).
- Achanta, R.S., Gill, W.N., and Plawsky, J.L., (2008) *J. Appl. Phys.*, **103**, 014907.
- 11) Achanta, R.S., Gill, W.N. and Plawsky, J.L., (2007) *Appl. Phys. Lett.*, **91**, 234106.

12) Achanta, R.S., Gill, W.N. and Plawsky, J.L., J. Appl. Physics, 106, 074906 (2009).