



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

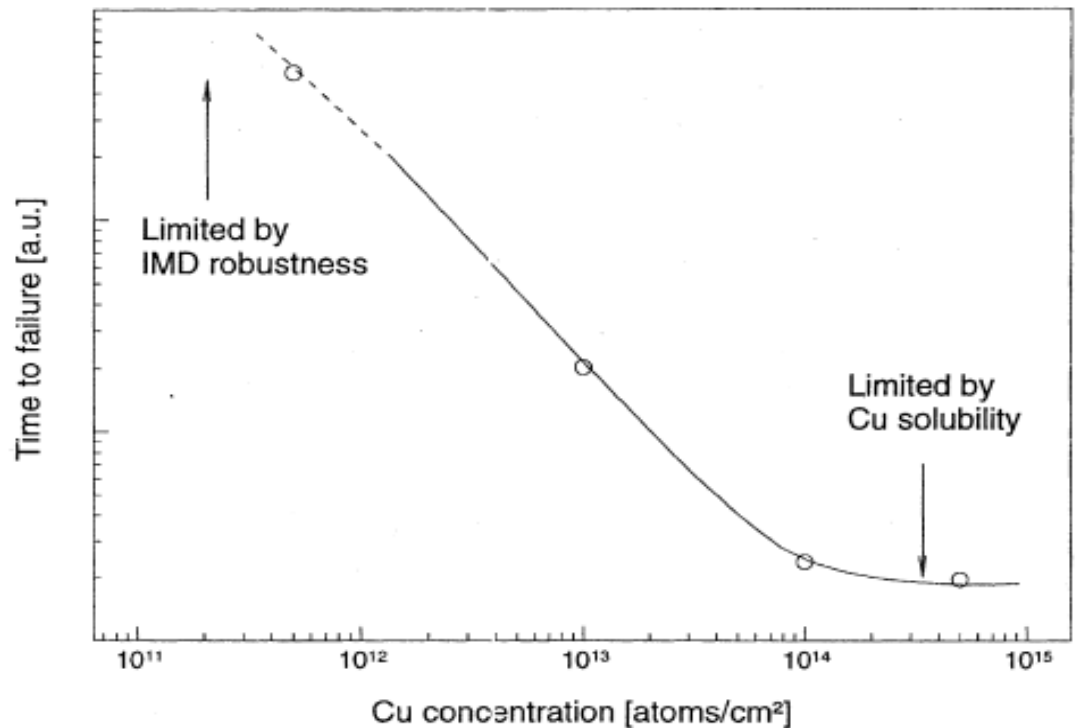
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Failure of Dielectrics Depends on the Concentration of Impurities

- Dielectrics can be in contact with a metal (Cu), a diffusion barrier (Ta, TaN, TiN, W, Al...) or a hard mask (Si nitride).
- Dielectrics and metals should be inert, but some interaction is necessary to promote adhesion.
- Reactions and diffusion needed for adhesion adversely affect the reliability of interconnect structures.
- Interactions are governed by reactions between the dielectric and the deposited film and the diffusion of injected material due to concentration gradients and an applied electric field.

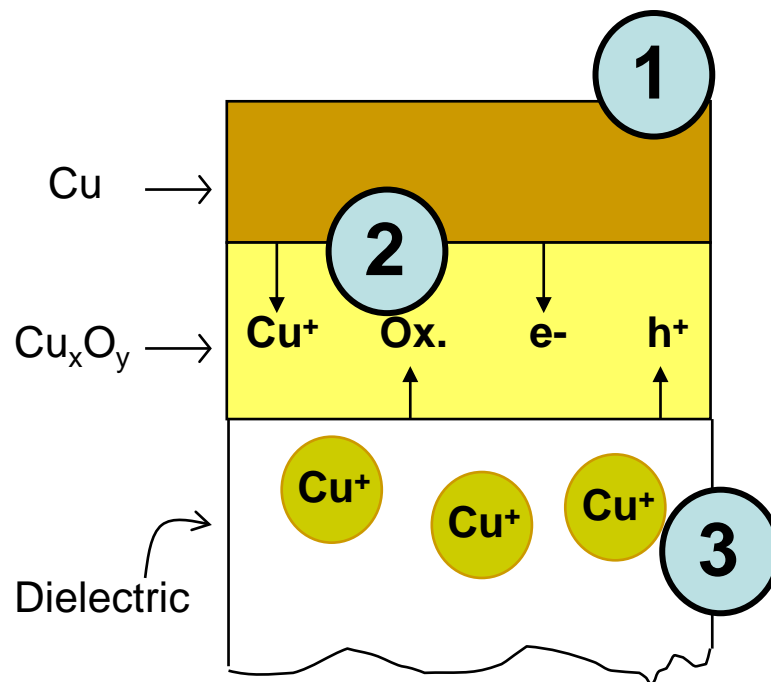


R.Gonella, *Microelectron.Engg.*55, 245, (2001)



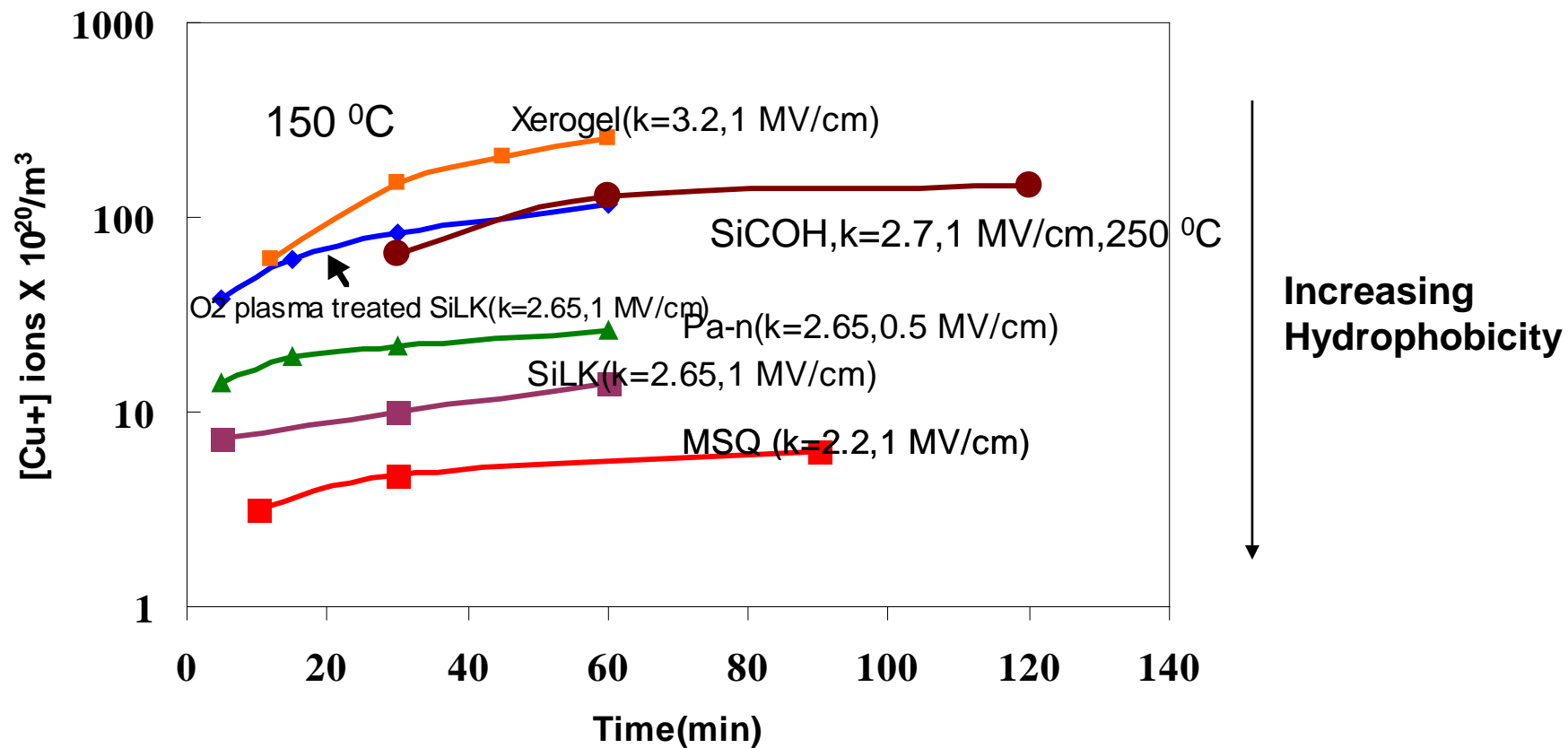
Our Proposed Cu Injection Mechanism

- Cu interacts with the interfacial oxygen and moisture to form non-stoichiometric oxide (Cu_xO_y)
- The combination of moderate temperatures ($< 300\text{ }^\circ\text{C}$) and an external electric field during operation may induce the breakdown of the copper oxide to ions.
- The Cu oxide, acts as the source of the Cu ions that are available for diffusion.
- Cu ions, driven by the applied field, drift through the dielectric.





Copper Injection Depends on the Hydrophilic Nature of the Dielectric



Increasing hydrophobicity leads to less metal ion injection.



Modeling Copper Ion Drift/Diffusion

- Species: Cu^+ ions
- Surface reaction to form Cu oxide and Cu ion source is very rapid.
- Cu^+ mass flux consists of thermal and field assisted diffusion (drift):

Continuity Equation

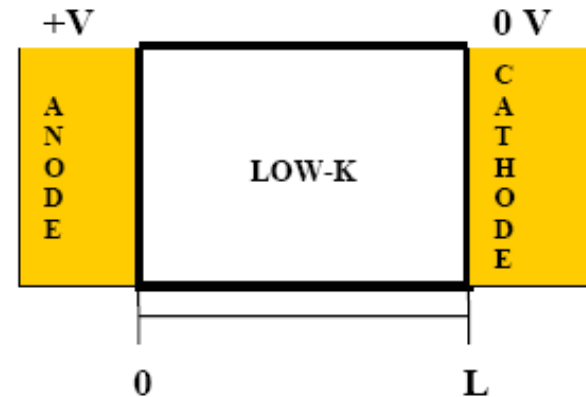
$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} + \mu \frac{\partial}{\partial x} C \frac{\partial V}{\partial x}$$

Poisson equation

$$\frac{\partial^2 V}{\partial x^2} = - \frac{qC}{k_D \epsilon_0}$$

Einstein Relation

$$\mu = \frac{qD}{kT}$$



Nomenclature

C : concentration of Cu^+

V : voltage

μ : mobility of species

D : diffusivity of Cu^+

k_B : boltzmann constant

q : elementary charge

k_D : dielectric constant

ϵ_0 : permittivity of vacuum

T : temperature



Boundary Conditions-Failure Criterion

- Initial Conditions:

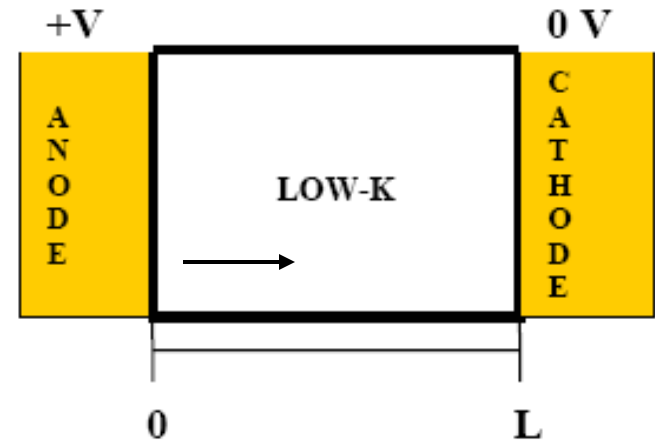
$$t = 0 \quad C(x, t) = 0 \quad V(0, t) = 0 \quad V(L, t) = 0$$

- Boundary Conditions:

$$x = 0 \quad C(0, t) = C_e \quad V(0, t) = V_o$$

$$x = L \quad V(L, t) = 0$$

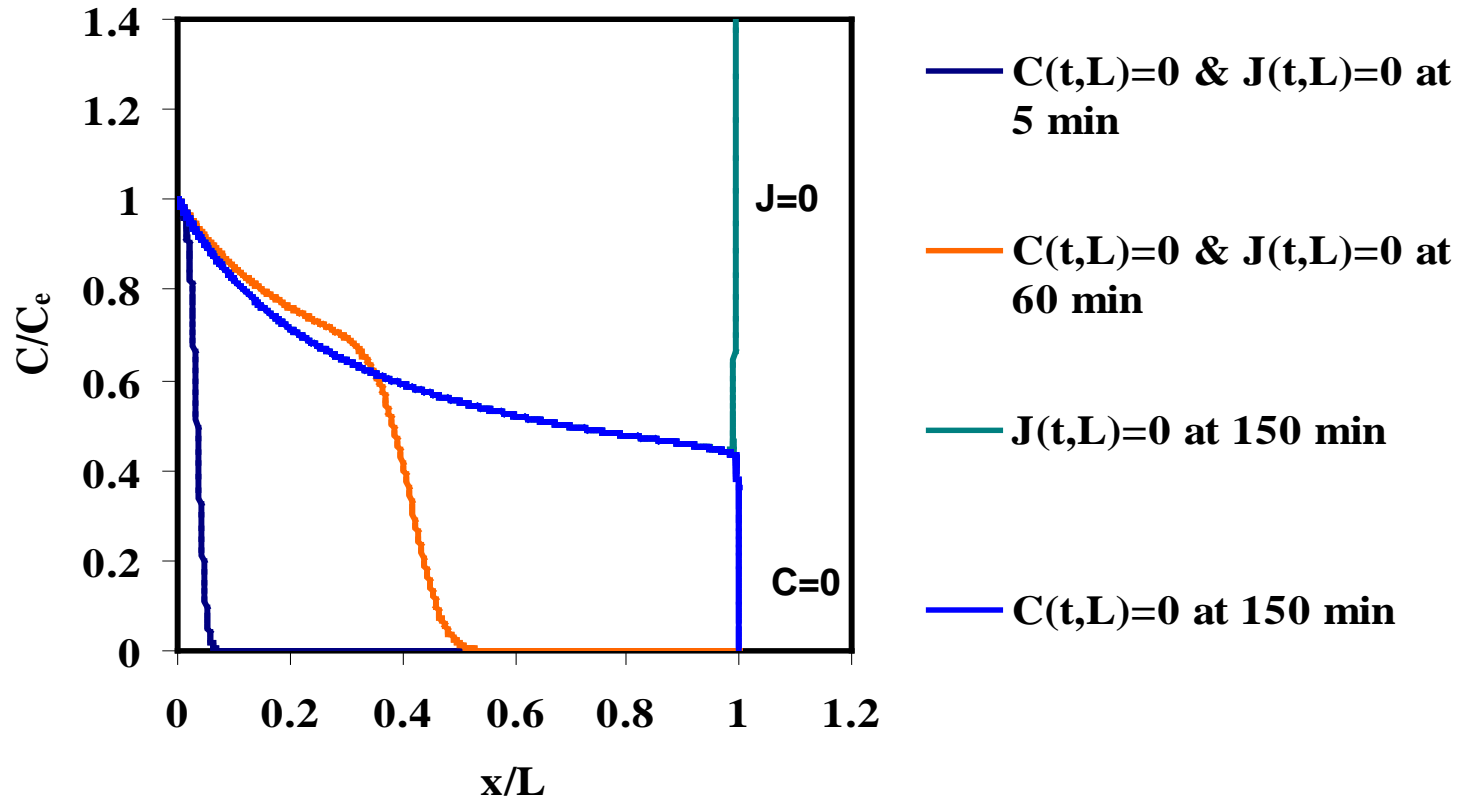
$$C(L, t) = 0 \quad \text{or} \quad J = -D \frac{\partial C}{\partial x} - \mu C \frac{\partial V}{\partial x} = 0$$



Failure is assumed when $E(L)$ exceeds intrinsic breakdown strength, E_{bd}



Concentration Profiles



Simulation parameters:

$$C_e=10^{17} \text{ at/cm}^3,$$

$$D=10^{-20} \text{ m}^2/\text{s},$$

$$T=250 \text{ }^\circ\text{C},$$

$$L=200 \text{ nm},$$

$$V_0=20 \text{ V},$$

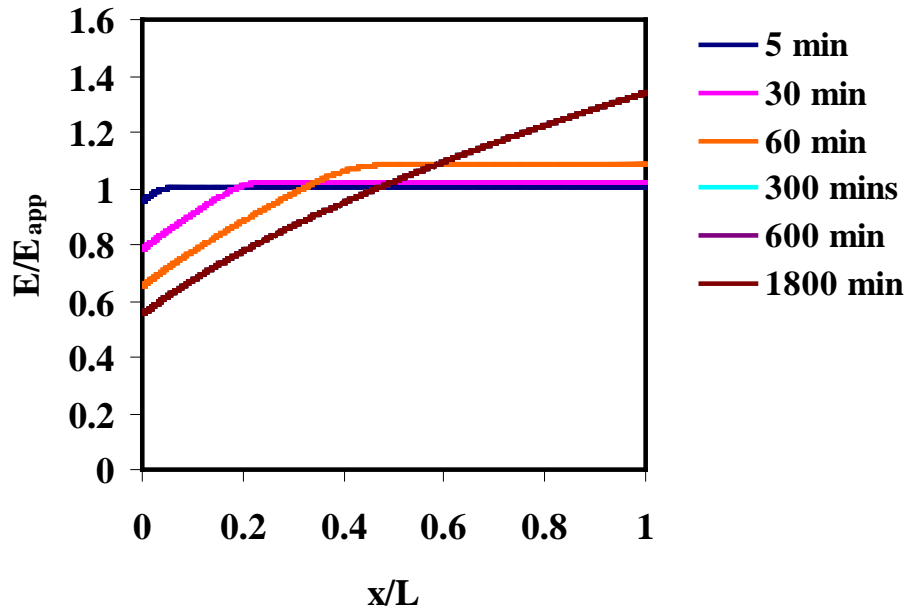
$$k_D=2.7,$$

$$E_{\text{app}}=1 \text{ MV/cm}$$

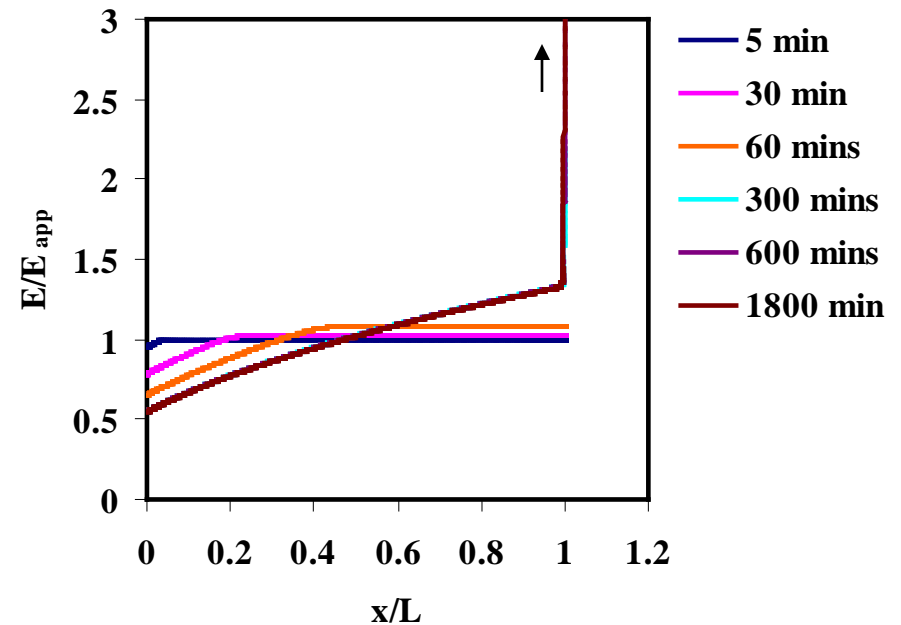


Electric Field Profiles

$C(t,L)=0$



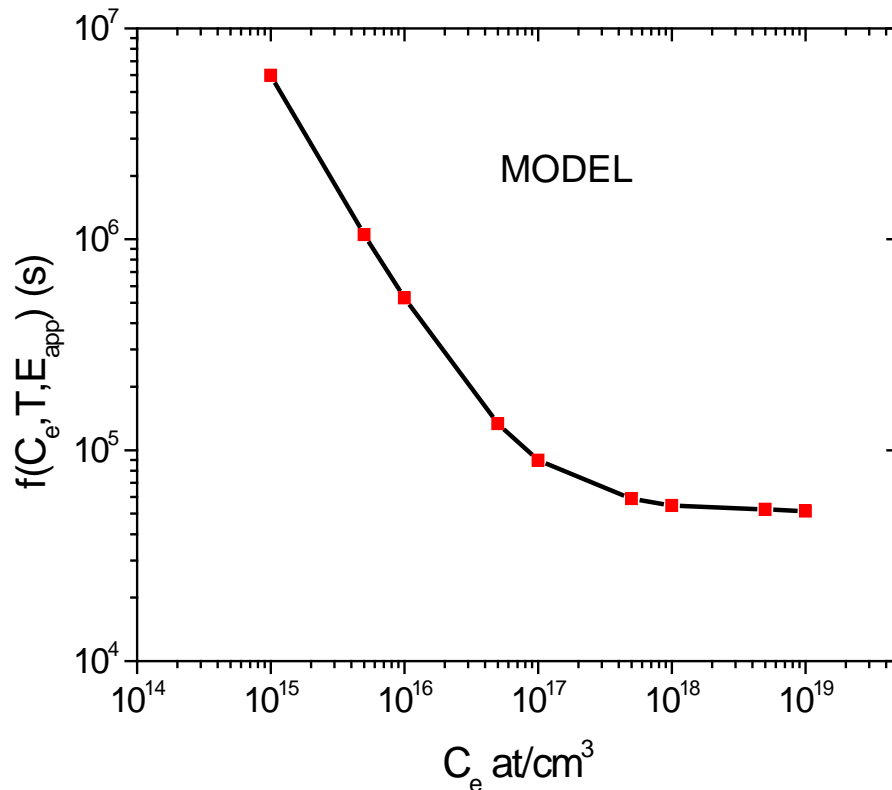
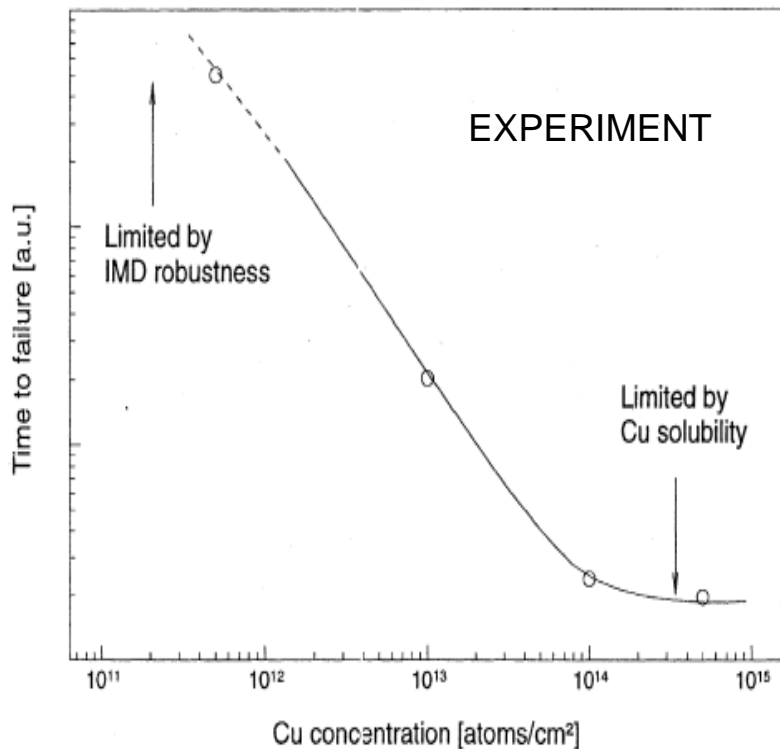
$J(t,L)=0$



- **Steady state quickly reached for $C(t,L)=0$.**
- **Field increase is significant only for $J(t,L) = 0$ boundary condition at $x=L$.**
- **Steady state is reached in the body of the dielectric but not at $x=L$ until long after breakdown for the $J(t,L)=0$.**



Mass Transfer Time $f(C_e, T, E_{app})$ vs C_e Curve Resembles Actual TTF Vs Cu Concn. Plot



Predicted model trends follow the actual trend in experimental data on time-to-failure for Metal/TEOS/Si capacitors.

Key Points: a) Solubility of dopant is critical b) Matching of experimental data shows that $J = 0$ boundary condition is the correct one.



Time to Failure-Intrinsic and Extrinsic Effects

- Mass transfer effects (diffusion) alone are insufficient to totally describe dielectric failure.
- Failure can arise due to exposure to high temperatures or exposure to high fields, even in the absence of a dopant like Cu. Mass transfer promotes failure and defines how failure depends upon impurities.
- Thermally activated mechanisms have an Arrhenius dependence on temperature. E_a is energy for bond disruption and diffusion vacancy creation. A is related to lattice vibrational frequency.

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

$$A = 2 - 70 \times 10^{-13}$$

$$E_a = 1.15 eV$$

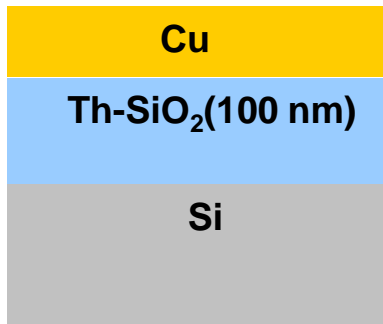
$$\gamma = 0.45 - 0.8$$

**Intrinsic “thermochemical”
effects**

Mass transfer effects



Considering Field Effect on Intrinsic Bond Breakage-After E-model



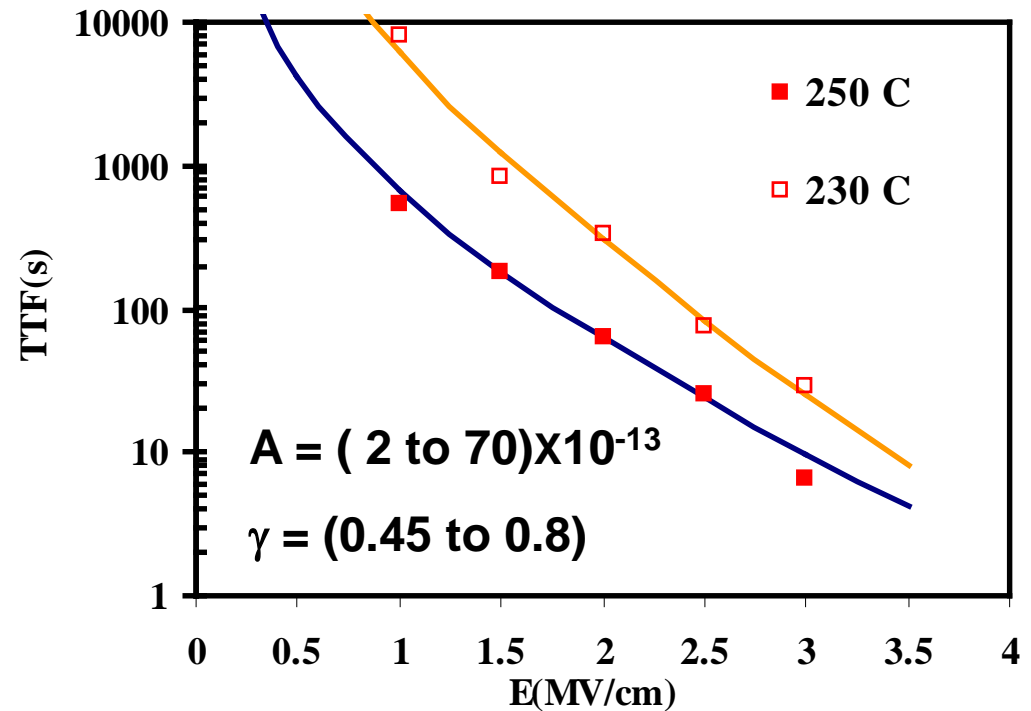
Model Parameters

$$C_e = 3 \times 10^{18} \text{ at/cm}^3$$

$$L = 100 \text{ nm}$$

$$k_D = 4$$

$$E_{bd} = 10 \text{ MV/cm}$$



- **Need improved theory to properly account for both temperature and electric field effect.**
- **Comsol simulation helped us to uncover the missing physics.**

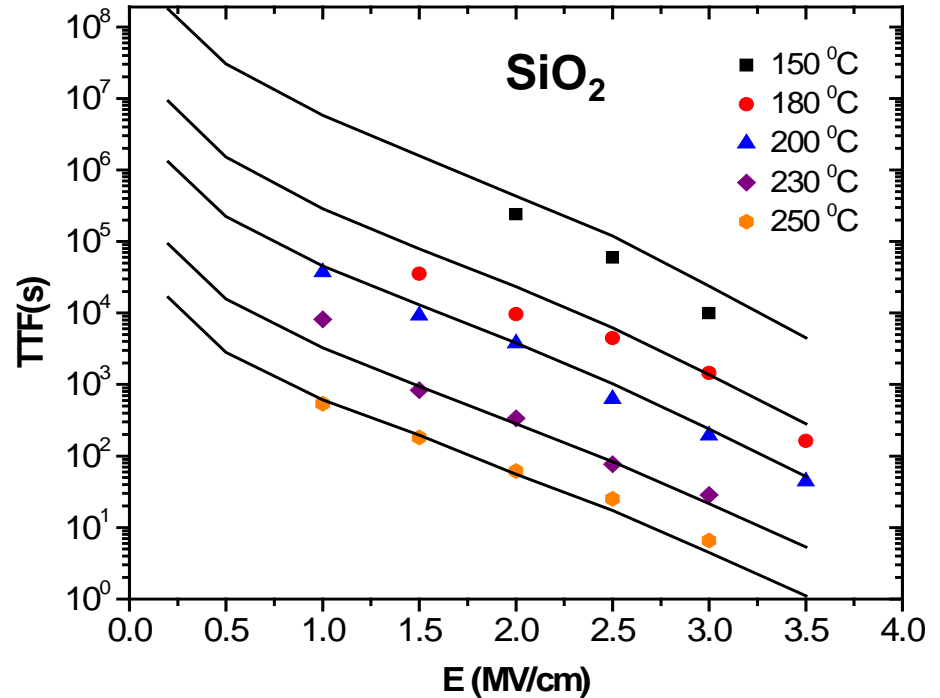


New Model Based on Physics: E_{app}^2 Dependence of Time to Failure

- The time to failure depends on E_{app}^2

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

- The induced dipole moment energy term (E^2 dependent) may be significantly higher than the permanent dipole moment energy term (E dependent) in the presence of copper ions.



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

Permanent dipole moment energy

Induced dipole moment energy

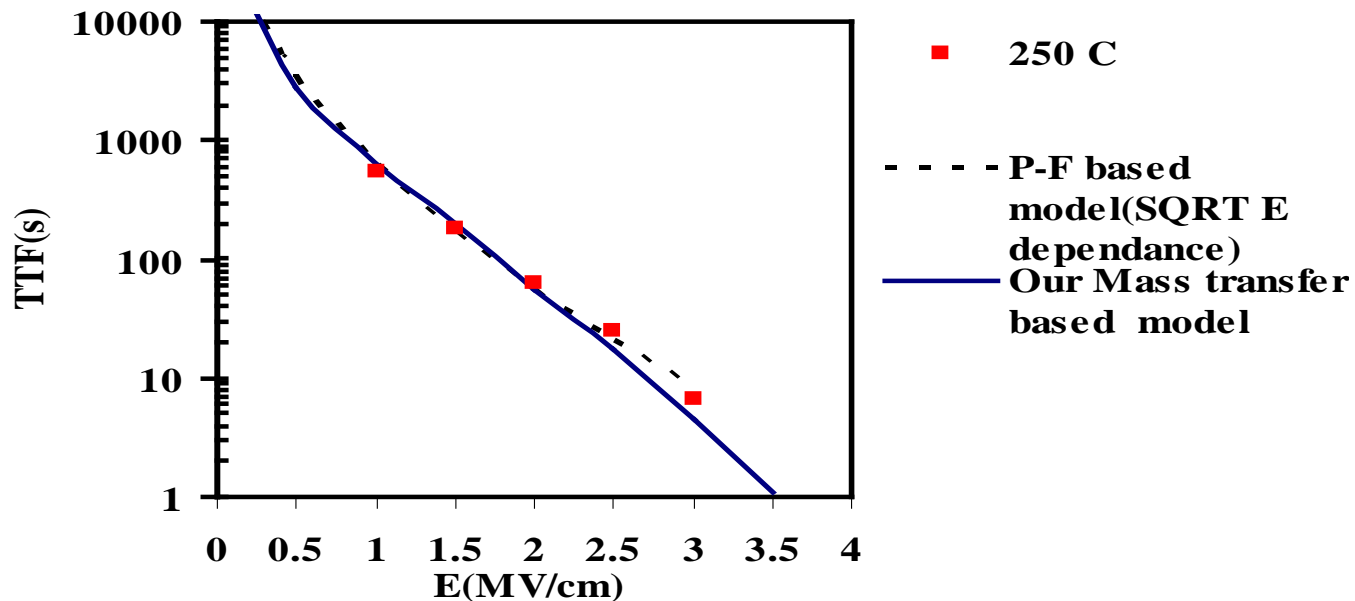
$$A = 2 \times 10^{-13}$$

$$\gamma = 0.015$$

$$E_a = 1.15$$



Mass Transfer Model and Poole-Frenkel Conduction Based Model



Mass Transfer Model

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

P-F conduction

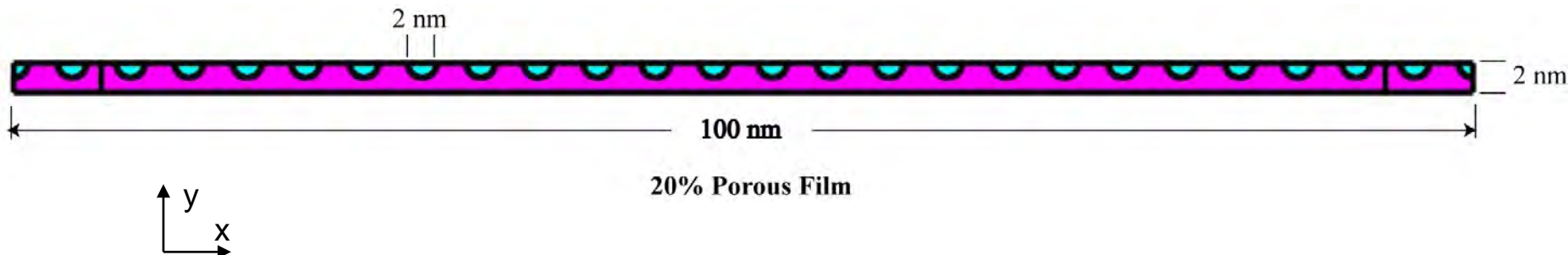
$$TTF(s) = \exp\left(12.3 - 5.87 \sqrt{E_{app}}\right)$$

Mass transfer model reproduces the low field effects described by the P-F formulation. P-F model requires different constants determined separately at each temperature



Nanoporous Materials Model

- Results from 1-D model prompted the development of a 2-D model with discrete pores.
- Incorporates the elastic drift formulation.
- Unit cell model, periodic in the y-direction with thickness, δ .
- The dielectric is 100 nm thick (L) with 2 nm pores ($2r_o$).
- Model considers a range of porosities from 0 - 50%.
 - No pore size dependence, yet.
- The pore dielectric constant can be varied independently of the matrix.





Model Equations - 2 or 3-D

- Continuity and Poisson's Equations

$$\frac{\partial C_{cu}}{\partial t} = -\nabla \mathbf{g} \left\{ -D_{cu} \left[1 + \left(\frac{\alpha_{cu}}{k_B T} \right) C_{cu} \right] \nabla C_{cu} - \mu_{cu} C_{cu} \nabla V \right\}$$

$$\nabla \mathbf{g} (k_D \varepsilon_o \nabla V) = q C_{cu}$$

Cu ions	(C_{cu})
Cu diffusivity	(D_{cu})
Cu elastic stress constant	(α_{cu})

- Initial and Boundary Conditions

$$t = 0 \quad C_{cu} = 0 \quad V = 0$$

$$x = 0 \quad C_{cu} = C_e \quad V = V_o$$

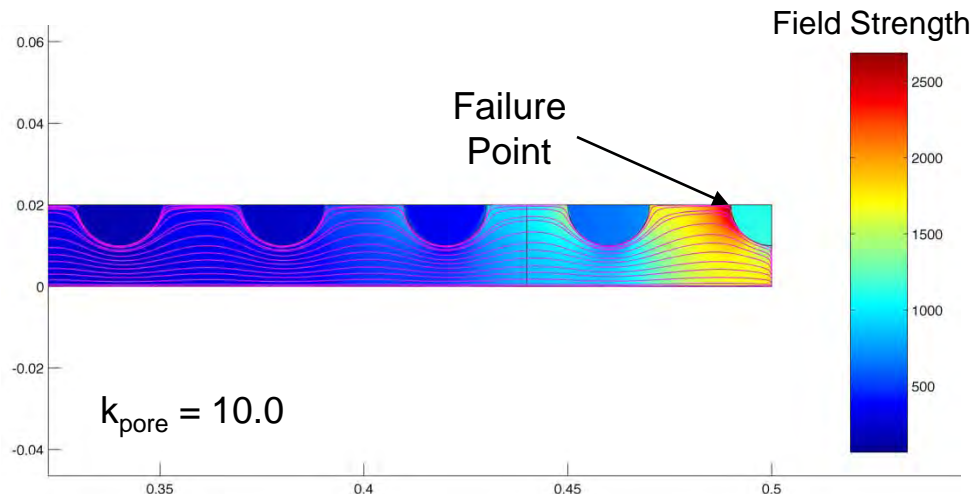
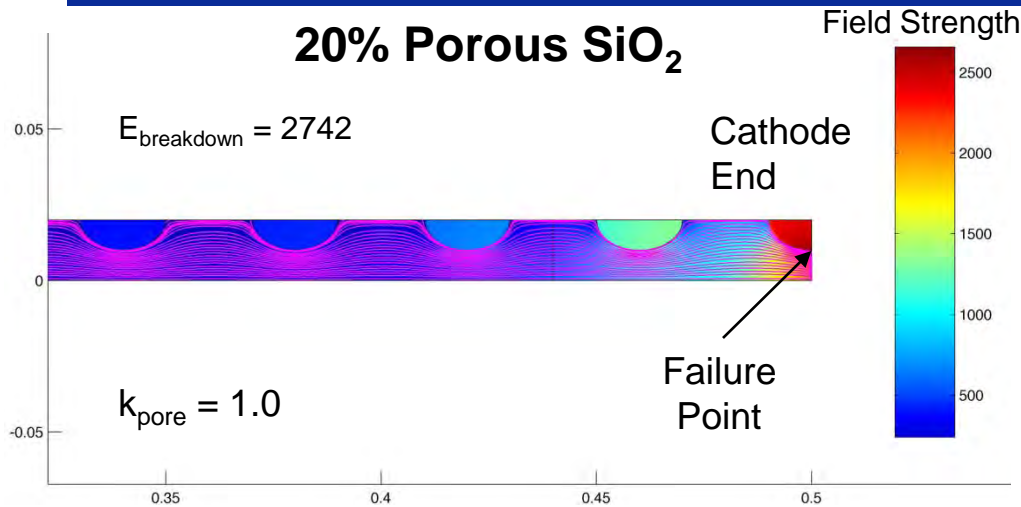
$$x = L \quad D_{cu} \left[1 + \left(\frac{\alpha_{cu}}{k_B T} \right) C_{cu} \right] \nabla C_{cu} + \mu_{cu} C_{cu} \nabla V = 0 \quad V = 0$$

$y = 0, \delta$ & pore surfaces

$$D_{cu} \left[1 + \left(\frac{\alpha_{cu}}{k_B T} \right) C_{cu} \right] \nabla C_{cu} + \mu_{cu} C_{cu} \nabla V = 0$$



Failure Location Depends on the Pore Dielectric Constant



- Failure location depends upon the effective pore dielectric constant.
- Failure always occurs somewhere on the pore surface where the field peaks.
- Ion flow streamlines (lavender) follow the contours of the pores and are concentrated near the surface of the pores.
 - Percolation path once failure occurs will follow along the surface of the pores.
- Simulations predict that the time-to-failure increases with increasing porosity.



Conclusions

- **New models were developed that tie the solubility and mass transfer of Cu in the dielectric and the thermochemical interaction of Cu ions with the dielectric to better explain and predict Cu enhancement of the time to failure.**
 - **Model successfully simulates and explains all the experimental data on SiO₂.**
 - **Comsol was instrumental in helping uncover the physics governing the process.**

- **The results of the new model offer testable hypotheses regarding the reason for Cu failure enhancement and directions for developing new dielectric and barrier materials.**

- **Next steps are:**
 - **2 and 3-D simulations incorporating negatively charged (moisture) species that form the Cu ions.**
 - **Anode reactions for the Cu ions**
 - **Adsorption/desorption of moisture from pores (weak form on pore boundaries).**
 - **Using Comsol predictions for failure to help guide experiments.**



Elastic Drift/Diffusion¹ Term-Accounting for High Concentrations

When the concentration of copper ions in the dielectric becomes very high, (i.e. when $C(x) \gg k_B T / \alpha$ where α is an elastic stress constant to account for the interaction between the ions and the dielectric and is $\sim 2 \times 10^{-44} \text{ J.m}^3$)¹ elastic drift /diffusion flux becomes important and should be included in the analysis

$$k_B T / \alpha = 3 \times 10^{17} \text{ at/cm}^3 @ 250 \text{ }^\circ\text{C}$$

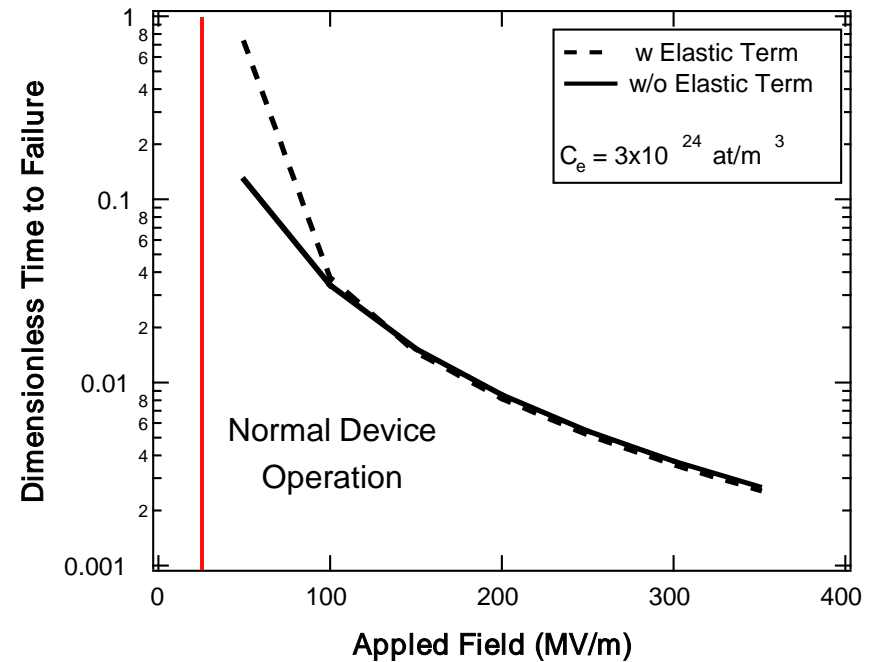
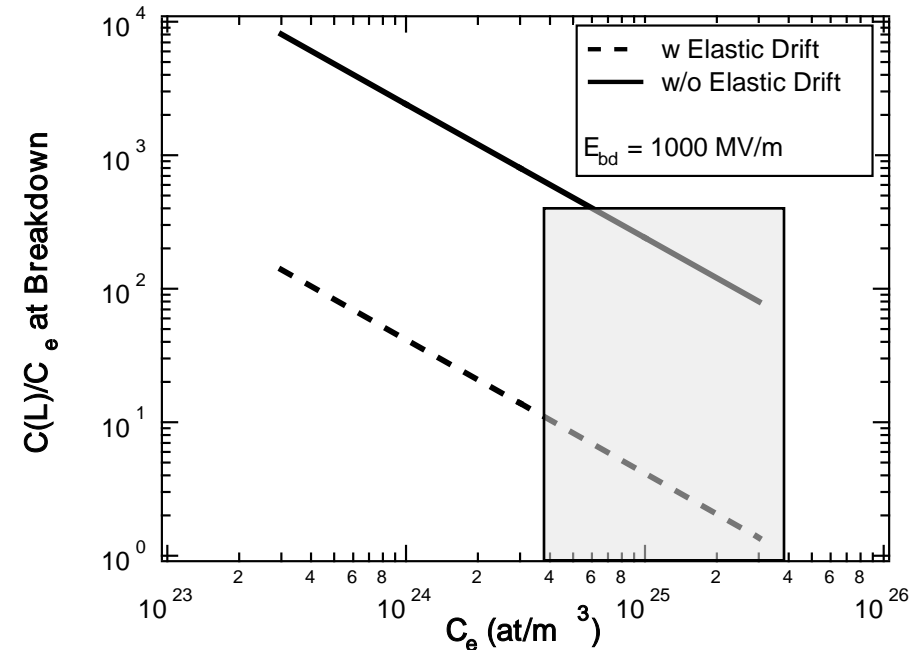
$$J(t, x) = -D \frac{\partial C}{\partial x} - \left(\frac{\alpha D}{k_B T} \right) C \frac{\partial C}{\partial x} - \mu C \frac{\partial V}{\partial x}$$



**Elastic drift/diffusion flux term
to account for “ion stuffing”**



Importance of Including Elastic Drift

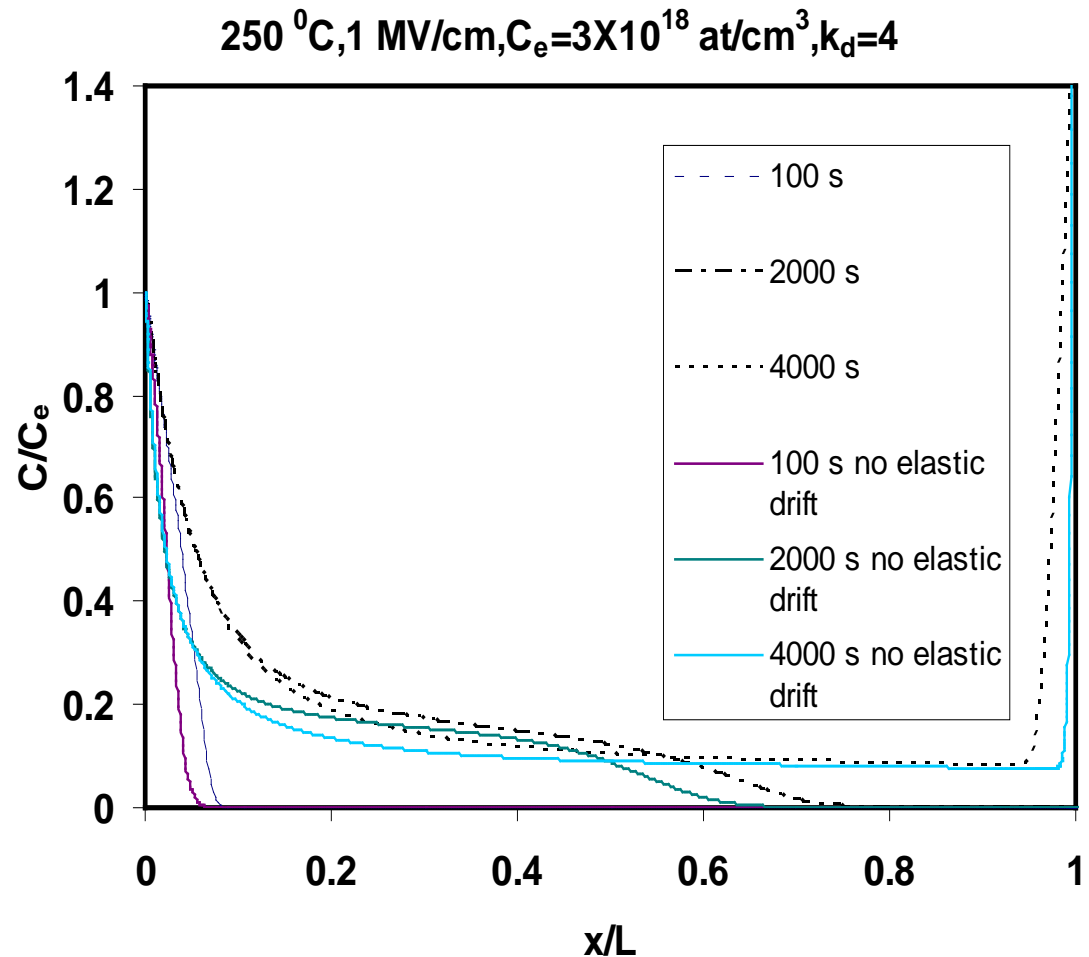


- Inclusion of elastic drift term causes a great change in the $C(L)$ without much effect on the time to reach breakdown.
- In the figure the solid line is without the elastic drift term while the dotted lines are with the elastic drift included in analysis.
- The shaded region represents the uncertainty in the value of C_e for SiO_2



Comparison: With and Without Elastic Drift/Diffusion

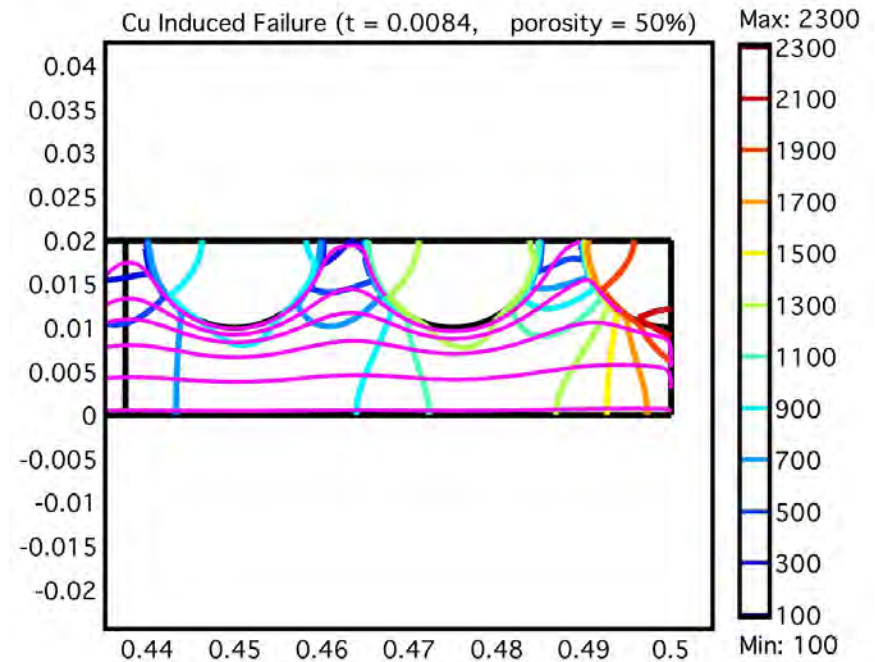
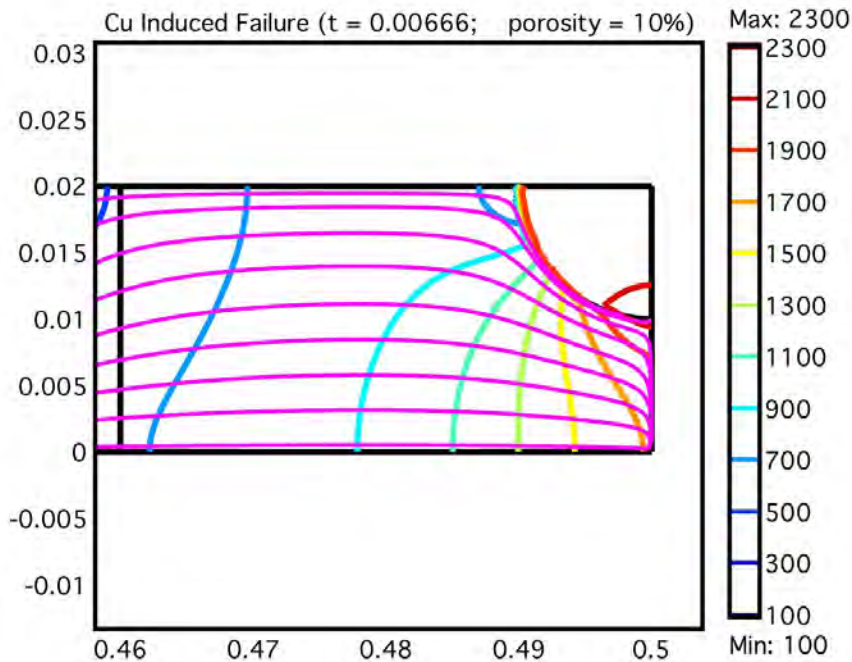
- Greater depth of penetration in the body of the dielectric with the elastic drift/diffusion term included.
- At the cathode ($x=L$) there is a greater back-drift of ions due to the additional elastic drift/diffusion term and steady state is quickly reached without too much build up of charge.
- At low applied fields (~ 0.4 MV/cm) the electric field at $x=L$, $E(L)$ never reaches E_{bd} as steady state is reached prior to it.



High field reliability testing may give erroneous estimate of lifetime at operating conditions



Porous Dielectrics– State at Breakdown



- Porous dielectrics will be used in future integrated devices. Manufacturers worry about premature failure.
- Model uses a unit cell approach with a 100 nm thick dielectric and 2 nm pores.
- Mass transfer model alone predicts an increase in time to failure with porosity due to a decrease in the mass flux through the solid (dry pores only).