Subcritical Cracking of Low-k Dielectrics

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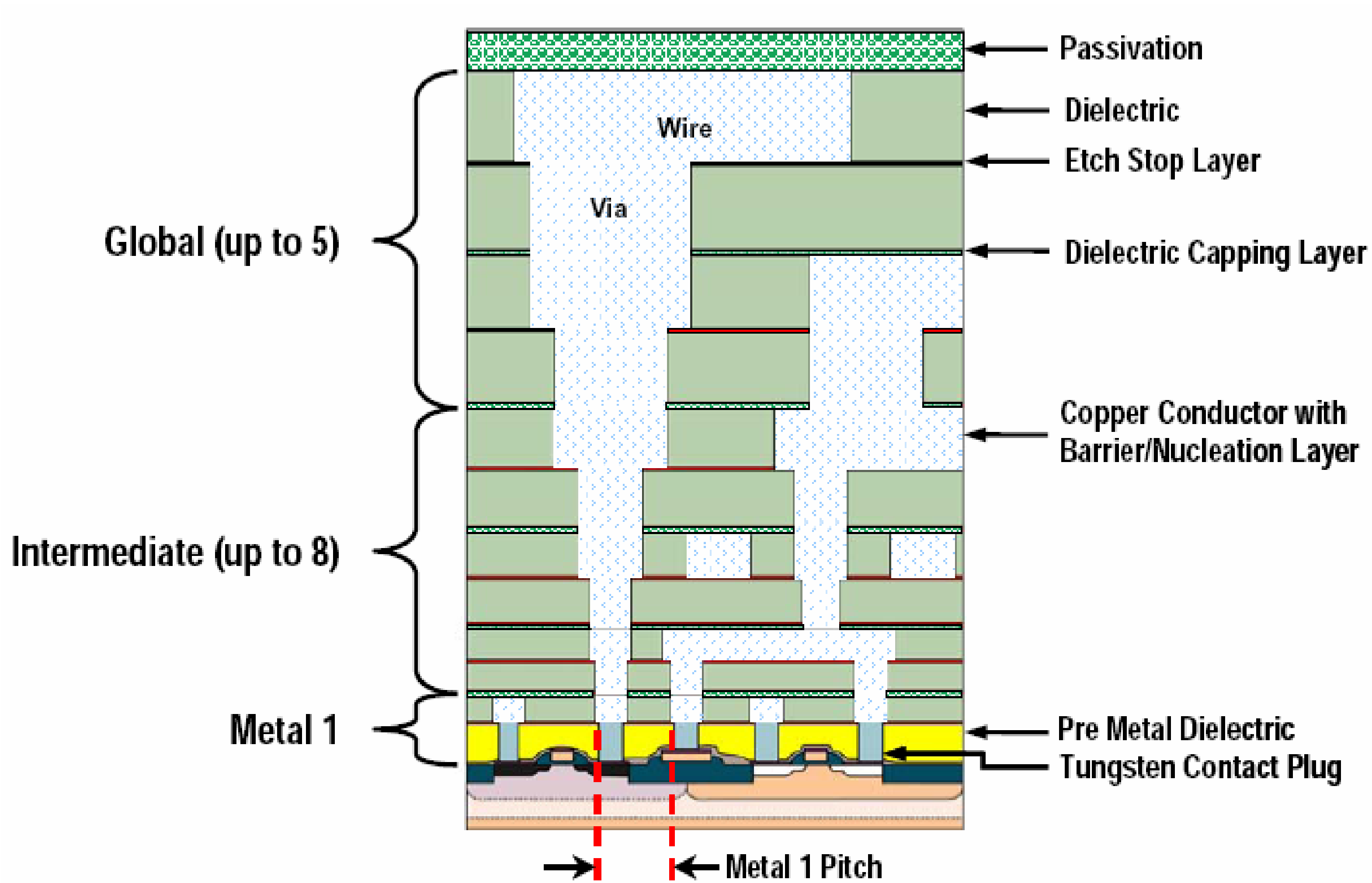
Fracture Mechanics, Spring, 2008

Outline

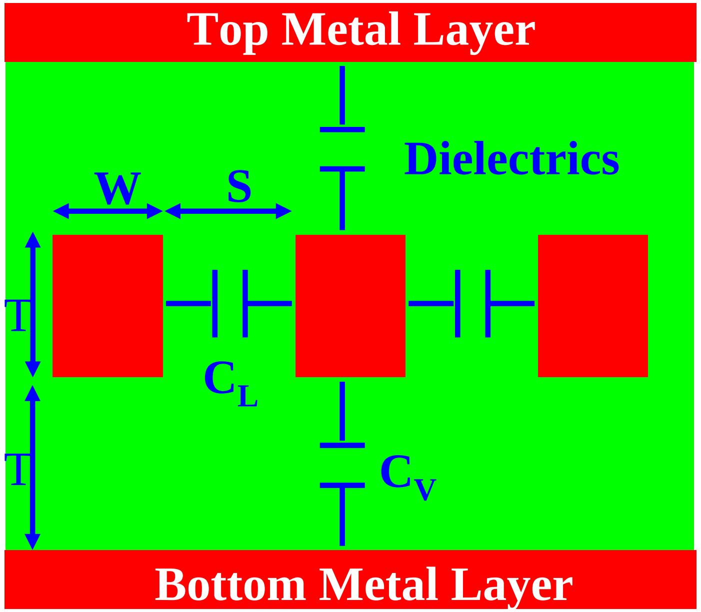
- ✓ Introduction of Low-k dielectrics
- ✓ Mechanistic study of subcritical crack
- ✓ Quantum chemical study of subcritical cracking

Multi-level Interconnect Structure



ITRS 2003 Interconnect, P8

Why Copper and Low-k



S.P. Jeng, et al, VLSI Tech. Symp. Tech.Dig. (1994) p73

R $= 2\rho L/PT$

C $= 2(C_L + C_V)$

$= 2\kappa\varepsilon_o(2LT/P + LP/2T)$

RC $= 2\rho\kappa\varepsilon_o(4L^2/P^2 + L^2/T^2)$

where

P $= W + S$

W $= S$

L = Line length

ρ = Resistivity

κ = Dielectric constant

Copper (ρ_{eff}=2.2μΩ·cm) and low-k (κ~2.0-3.0) are introduced to replace the conventional Al and SiO_2 for reduced RC delay in interconnect.

Approaches to Low k Dielectrics

✓ Reduce Bond Polarization ⇨

Incorporation of $-CH_3$ for weaker polarizability of C-H, Si-CH_3 relative to Si-O

✓ Reduce Bond Density ⇨

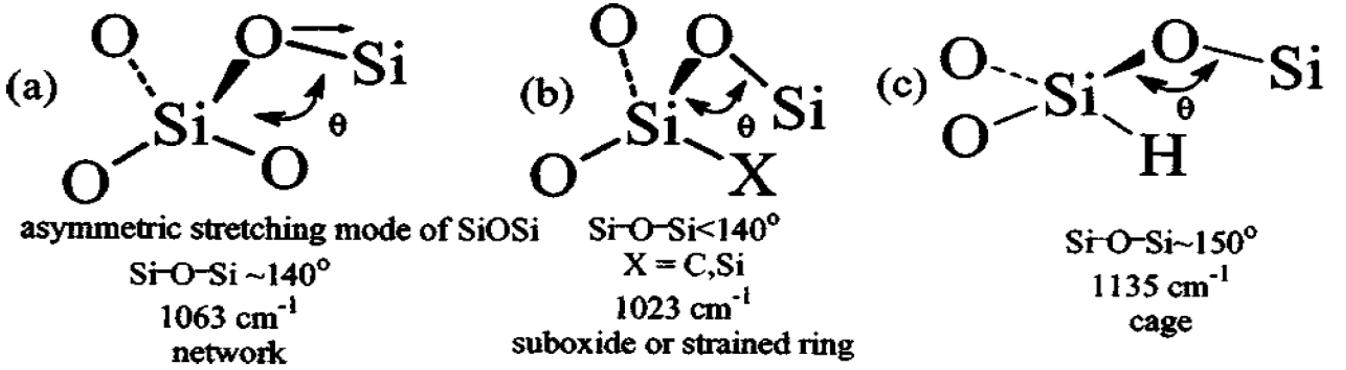
Incorporation of terminal organic groups

Introduction of porosity (air-gap as the most radical proposal)

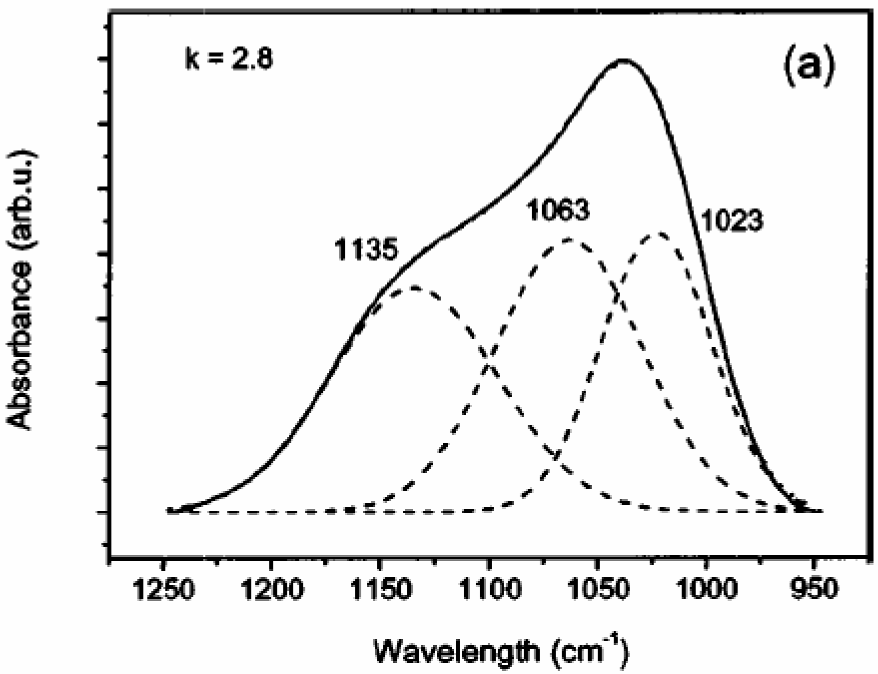
Organosilicate low k dielectrics (OSG) have been selected as the low k candidates.

Michael Morgen, Paul S. Ho, et al, Annu. Rev. Mater. Sci. Vol. 30, 645-680 (2000)

Variation of Si-O-Si Bond Angle in OSG



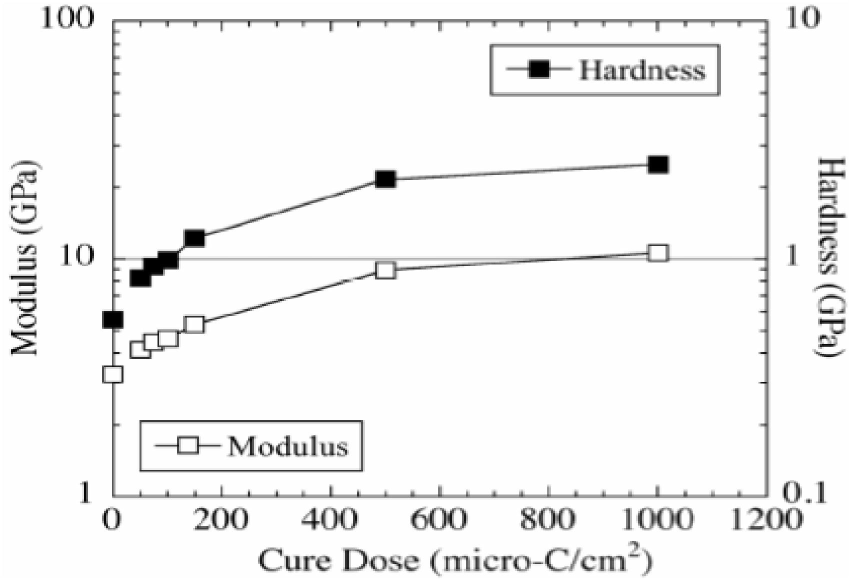
Alfred Grill and Deborah A. Neumayer, J. Appli. Phys., Vol. 94, No. 10, 6697-6707, 2003

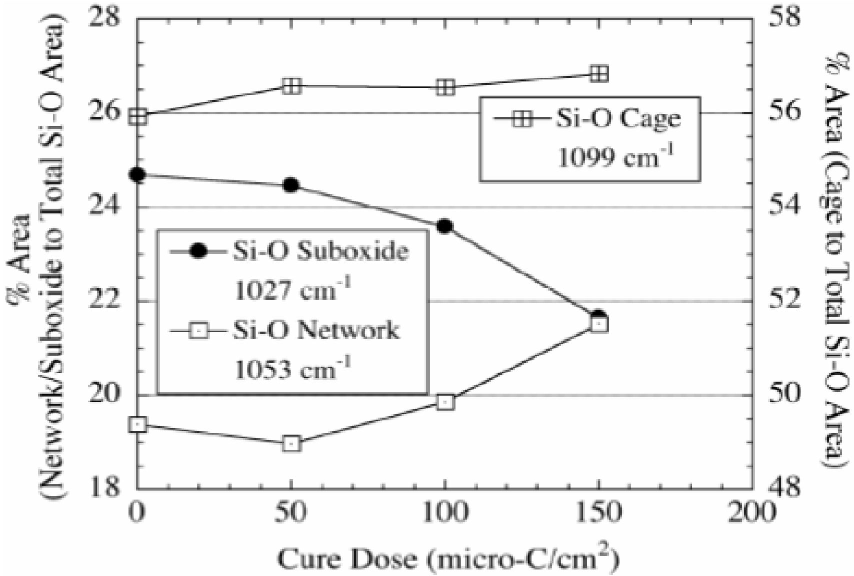


1023 cm^{-1}	1063 cm^{-1}	1135 cm^{-1}
Suboxide or strained ring	Network	Cage
Si-O-Si<140°	Si-O-Si~140°	Si-O-Si~150°

Fourier transform infrared spectroscopy (FTIR) characterization results

Mechanical Property and Bonding Configurations





Electron beam (EB) curing increases the hardness and modulus by forming more crosslinked Si-O structures at the expense of -CH_3 depletion.

Jeannette M. Jacques, Ting Y. Tsui, and Robert Kraft, etc. Mater. Res. Soc. Symp. Proc. Vol. 863 B3.8.1 2005

Challenges for Low-k

- ✓ **Materials challenges**

  Top issue for ultra low k integration: mechanical strength

  Decreasing elastic modulus and hardness with k

  Decreasing cracking resistance (cohesive strength) with k

- ✓ **Process related issues**

  Chemical Mechanical Polishing (CMP)

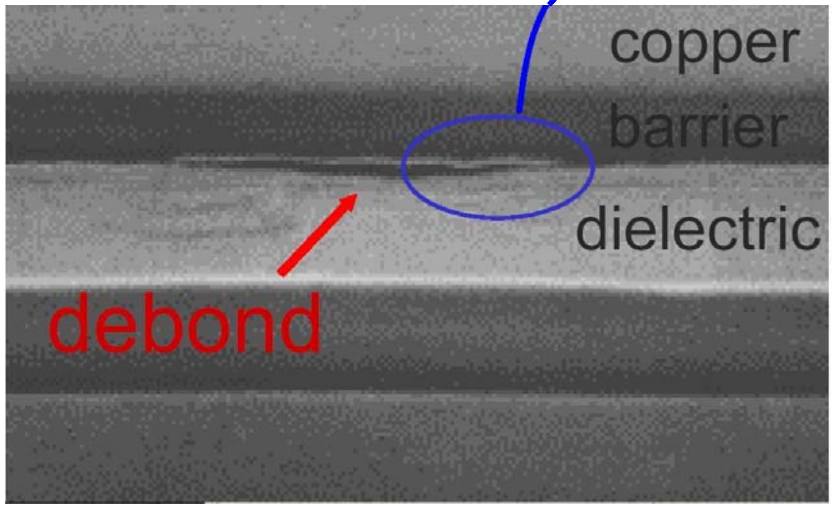
  Plasma damage

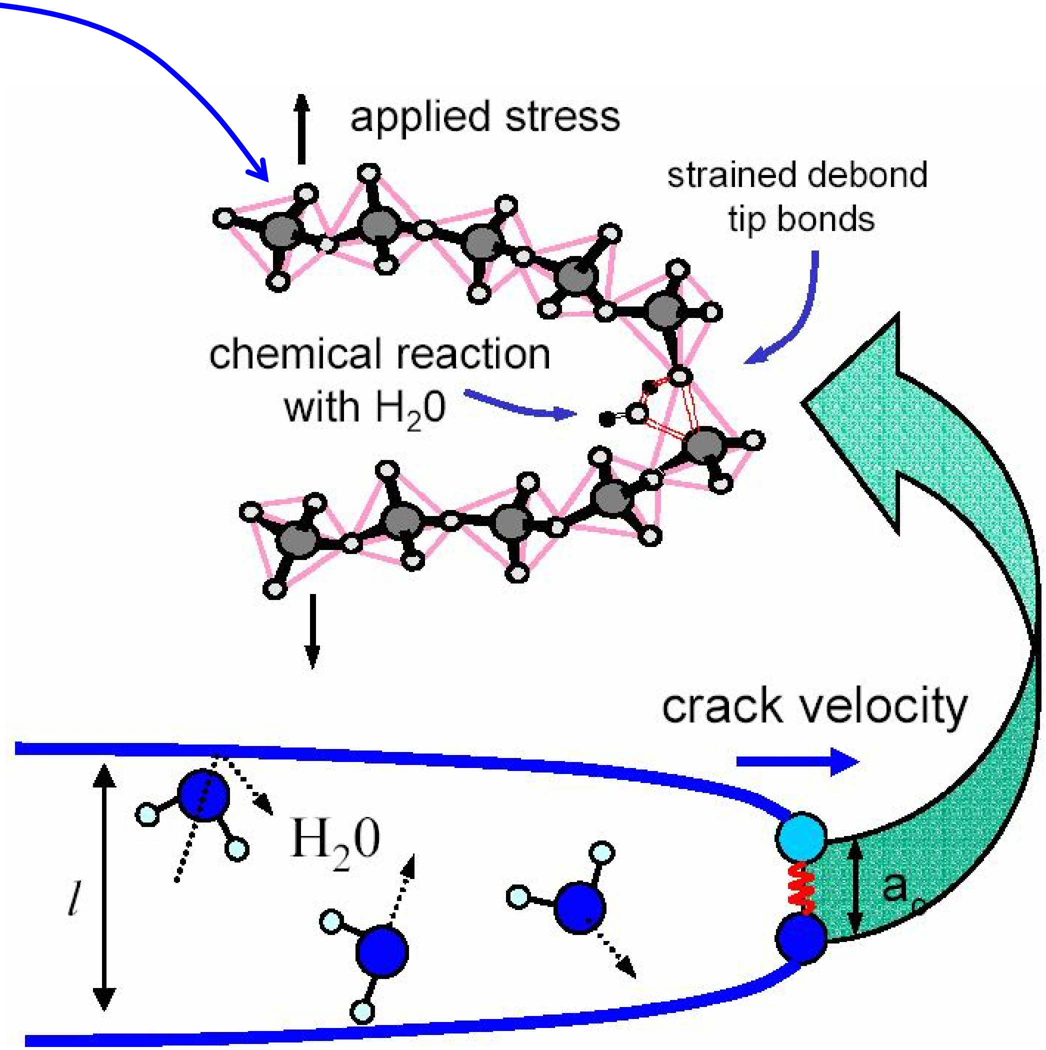
  Pore sealing

The material issue is further aggravated by stress corrosion , degradation of the material resistance against cracking under the combined influence of stress and environment such as relative humidity (RH) and potential of hydrogen (PH).

R. J. O. M. Hoofman et al. Microelectronic Engineering 80 (2005) 337-344

Moisture Assisted Subcritical Debonding

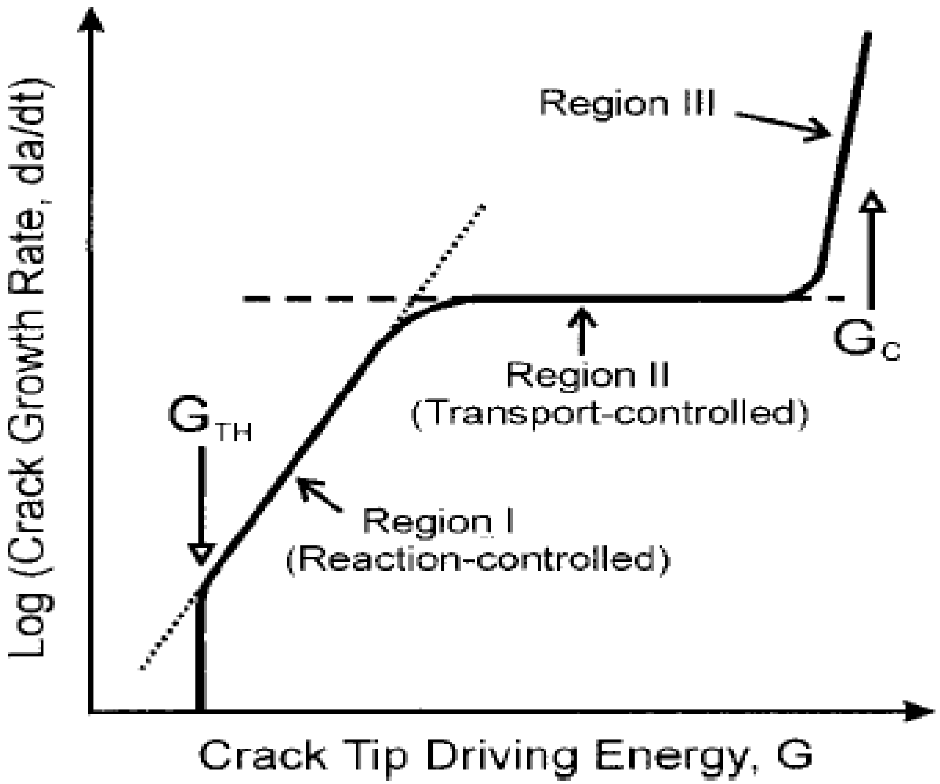




Adsorbed H_2O hydrolyzes stressed Si-O bonds and reduces fracture resistance. Subcritical debonding is important for reliability

M. Lane and R. H. Dauskardt – Proc. MRS, 1999

Subcritical Fracture



- † **Threshold energy release rate, G_{Th}**
- **I. Reaction-controlled region**
- **II. Transport-controlled region**
- **III. Catastrophic failure**

S. Kook and R. H. Dauskardt, J. Appl. Phs., Vol. 91, 1293-1303, 2002

Reaction-controlled Region

Model by Wiederhorn (1967), Lawn (1975), Cook & Liniger (1992), M. Lane (1999)

$$A + nX \leftrightarrow AX_n^* \leftrightarrow B$$

$$\Delta F = (\mu_B - \mu_A - n\mu_X)N = 2\gamma$$

$$\Delta\overrightarrow{G^*} = \Delta\overrightarrow{G_0^*} - \frac{\beta G}{N}, \quad \Delta\overleftarrow{G^*} = \Delta\overrightarrow{G_0^*} + \frac{(1-\beta)G}{N}$$

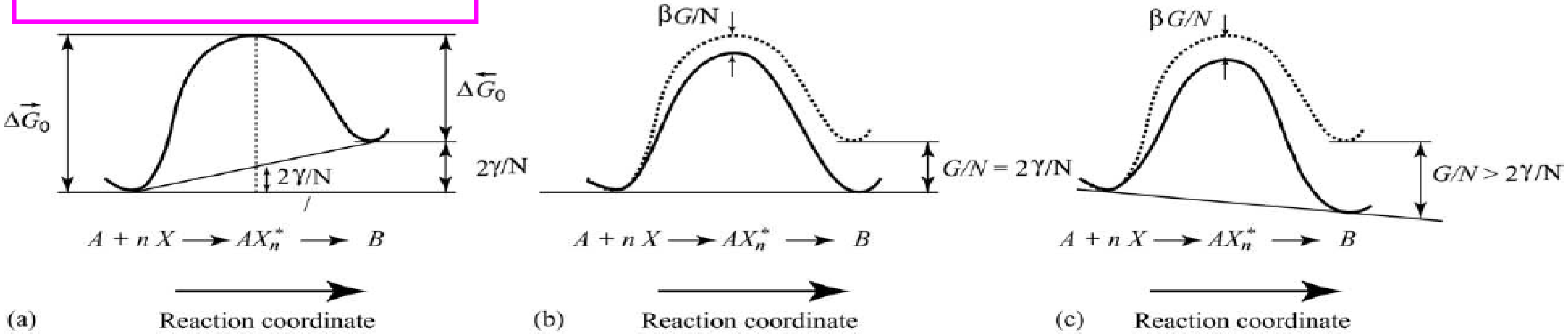
$$\omega = \omega_0 \left\{ \exp(-\frac{\Delta\overrightarrow{G^*}}{kT}) - \exp(-\frac{\Delta\overleftarrow{G^*}}{kT}) \right\}$$

$$v = v_0 \sinh(\frac{G - 2\gamma}{2NkT})$$

2γ: Intrinsic resistance to bond rupture

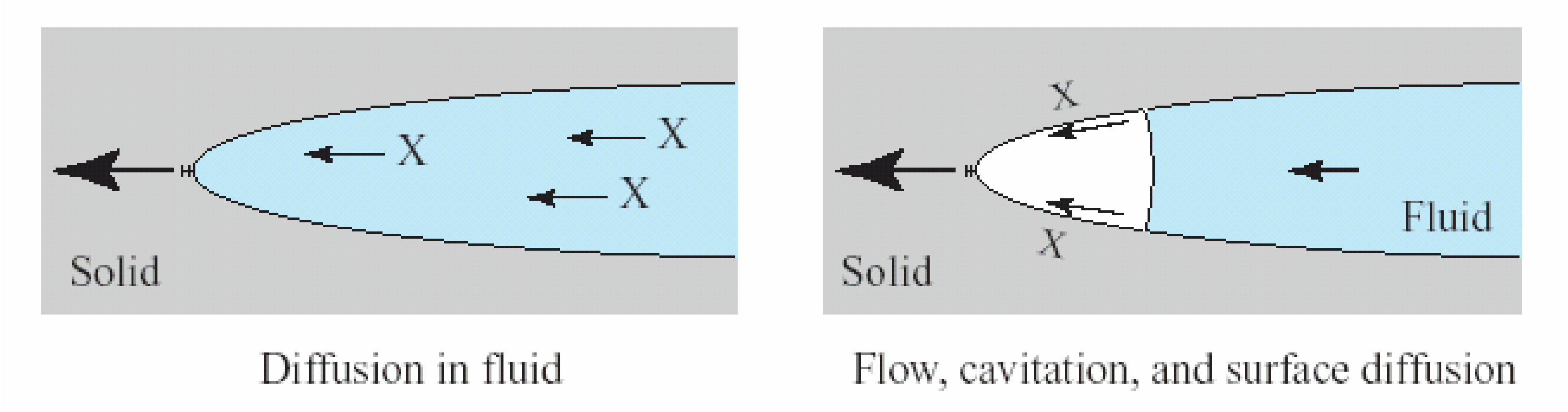
N: Bond density

J. J. Vlassak, etc., Materials Science and Engineering A 391 (2005) 159-174



G=0, no crack | **Threshold** | **Reaction control**

Transport-controlled Region



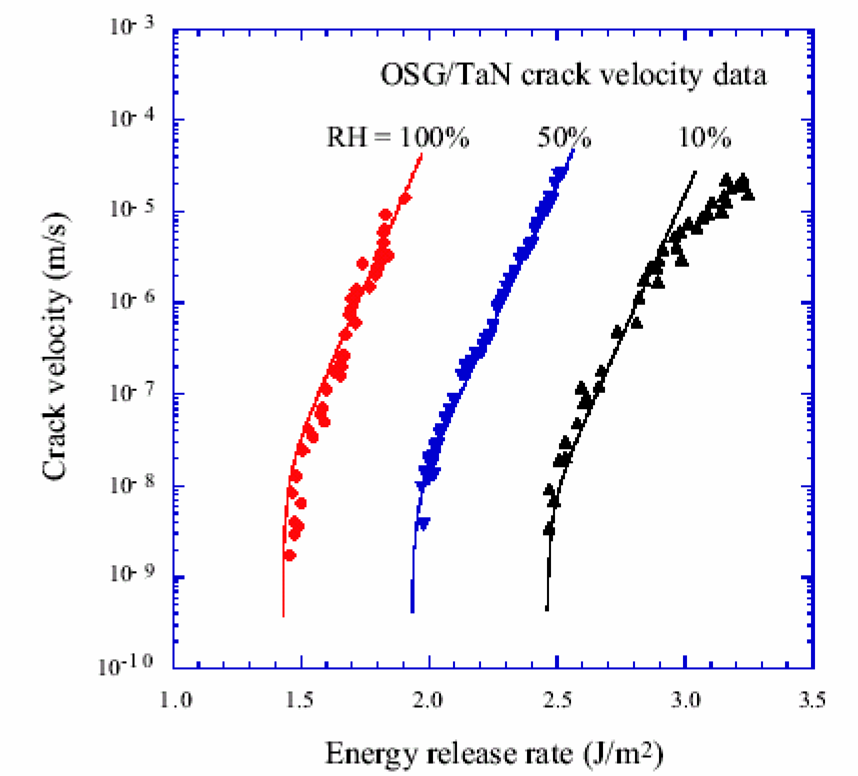
Flow limited:

$$p(x) = p_a - \frac{3\pi\mu v_3 E}{8G\left(1-\nu^2\right)} \ln\left(\frac{c}{x}\right)$$

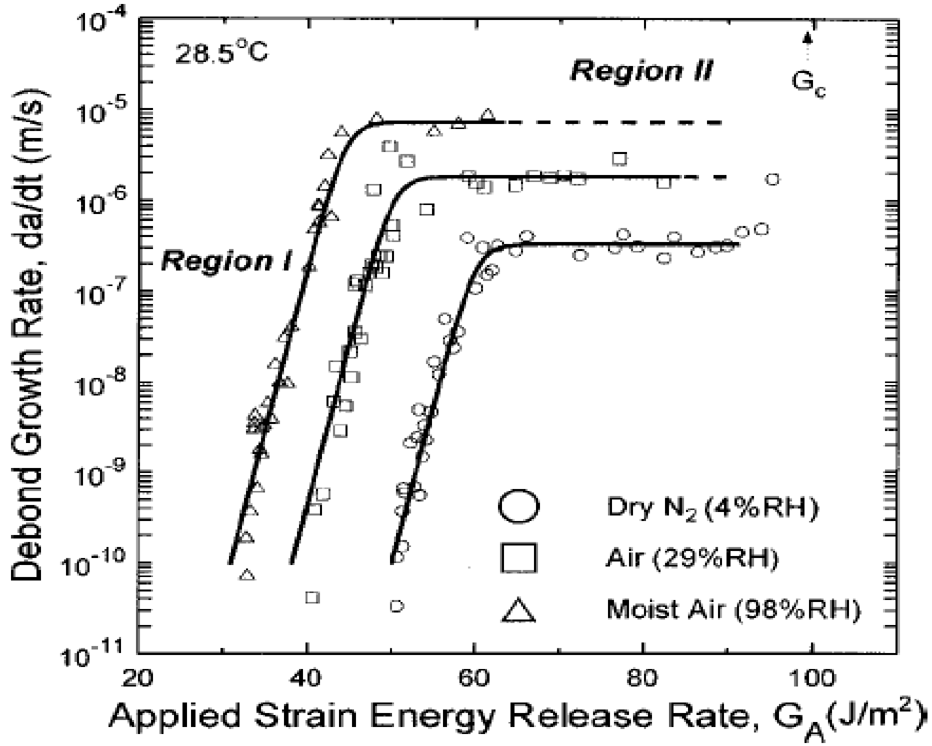
$$v_3 = \zeta \frac{8G\left(1-\nu^2\right) p_a}{3\pi\mu E} \sim 10^{-3}\ m/s$$

J. J. Vlassak, etc., Materials Science and Engineering A 391 (2005) 159-174

Effect of RH on Subcritical Crack Growth



J. J. Vlassak, etc., Materials Science and Engineering A 391 (2005) 159-174



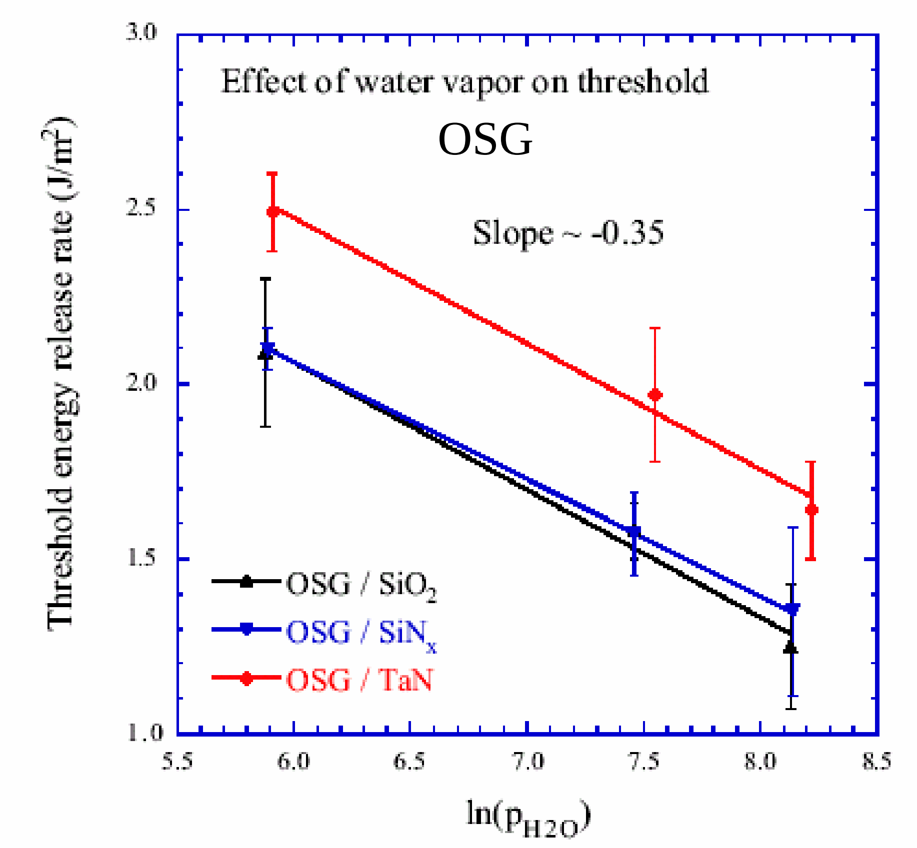
S. Kook and R. H. Dauskardt, J. Appl. Phs., Vol. 91, 1293-1303, 2002

Region I: $v = v_0 Sinh\left(\frac{G - 2\gamma}{2NkT}\right)$

Region II: $(\frac{da}{dt})_{II} = \frac{HD_{H_2O}}{L}(\frac{P_{H_2O}}{P_0})$

⇨ **N: ~ 8.6 x10^{18} m^{-2}**

Effect of RH on Threshold



$$Si-O-Si+nH_2O \leftrightarrow 2Si-OH$$

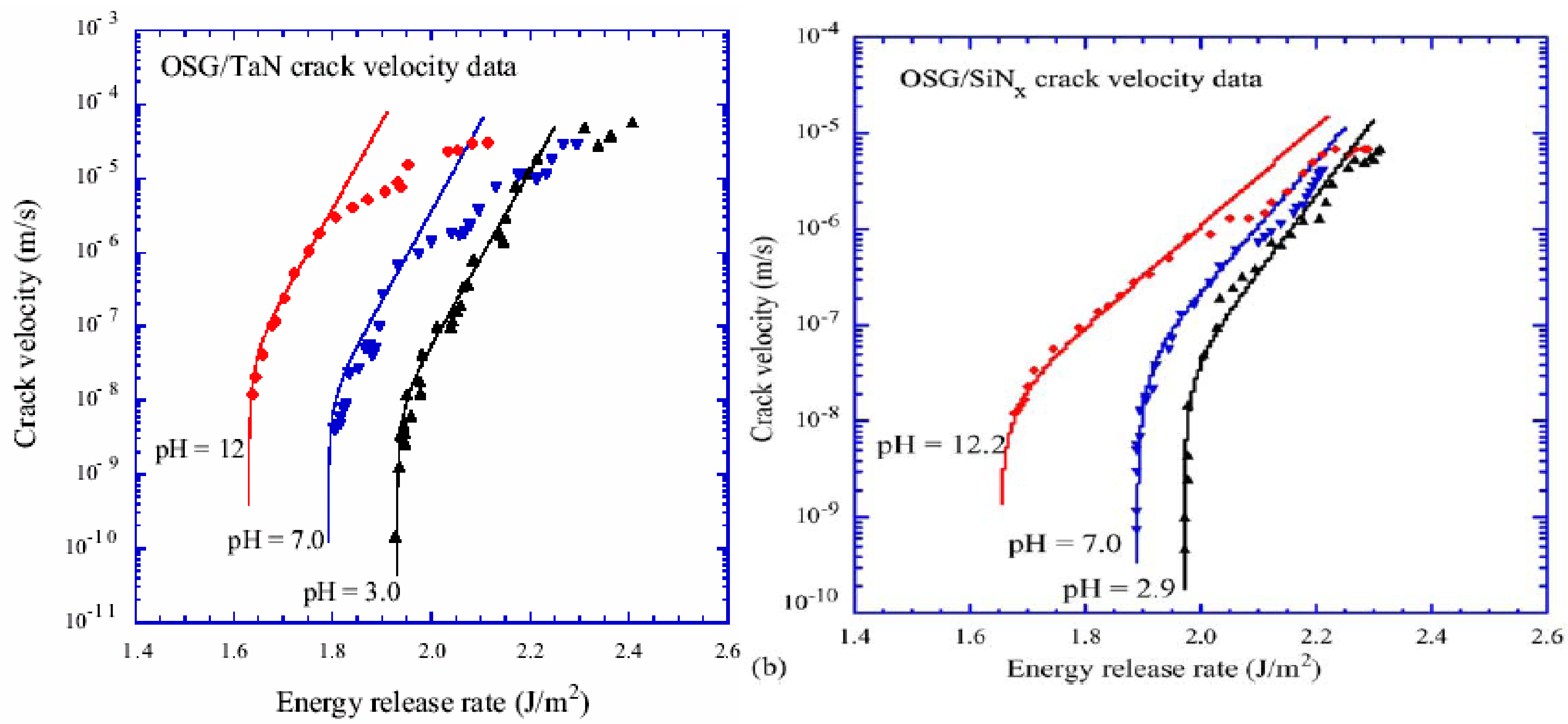
$$2\gamma = N(2\mu_{Si-OH} - \mu_{Si-O-Si} - n\mu_{H_2O})$$
$$= N\left[\Delta\mu - nkT\ln p_{\mathrm{H_2O}}\right]$$

⇨ **n~ 10**

Linear relationship between threshold energy release rate and natural logarithm of the water partial pressure.

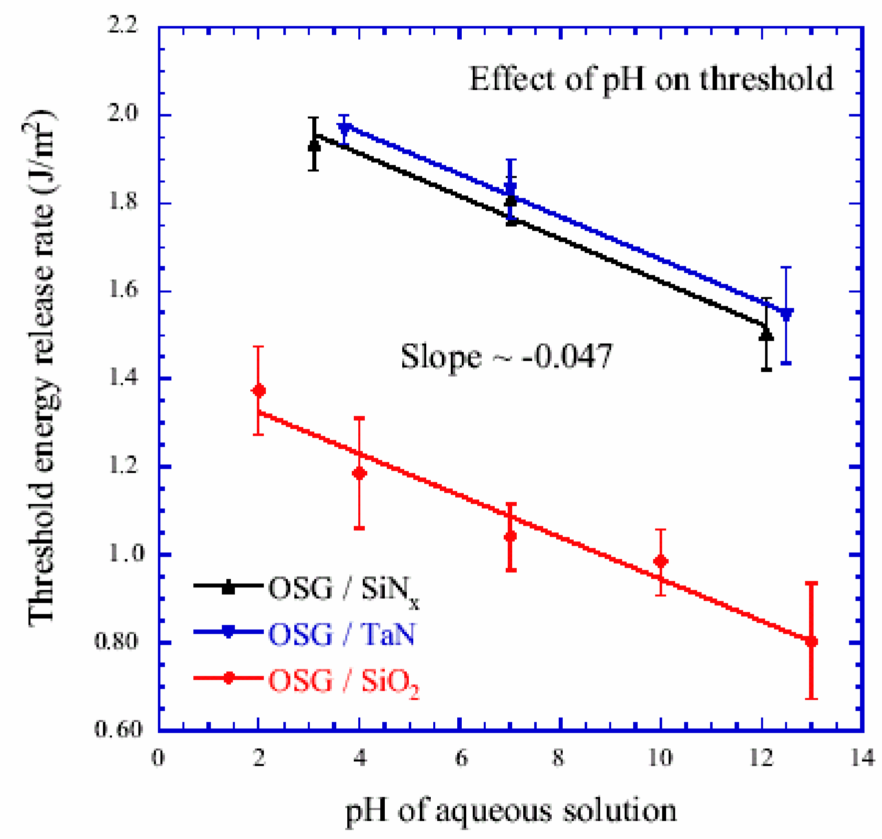
J. J. Vlassak, etc., Materials Science and Engineering A 391 (2005) 159-174

Effect of PH on Subcritical Crack Growth



J. J. Vlassak, etc., Materials Science and Engineering A 391 (2005) 159-174

Effect of PH on Threshold



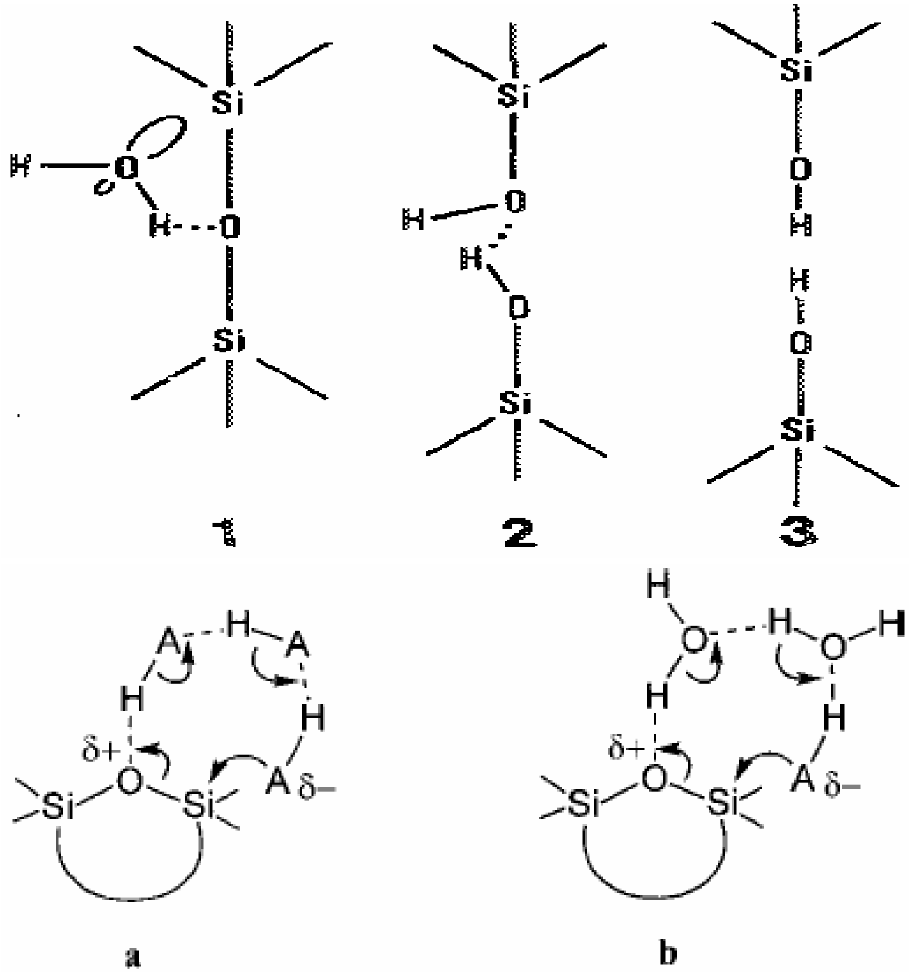
$$nOH^{-} + Si\text{-}O\text{-}Si \leftrightarrow Si - O^{-} + \text{Si-OH}$$

$$2\gamma = N\left[\Delta\mu + 14nkT\ln 10 - nkT\ln 10\, pH\right]$$

⇨ **n~0.56±0.07**

J. J. Vlassak, etc., Materials Science and Engineering A 391 (2005) 159-174

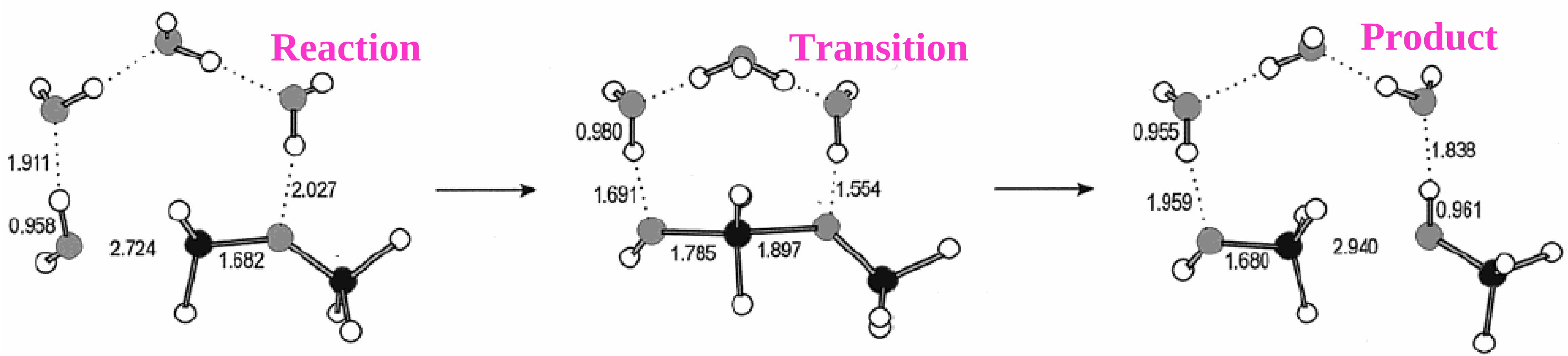
Michalske-Freiman (MF) Model

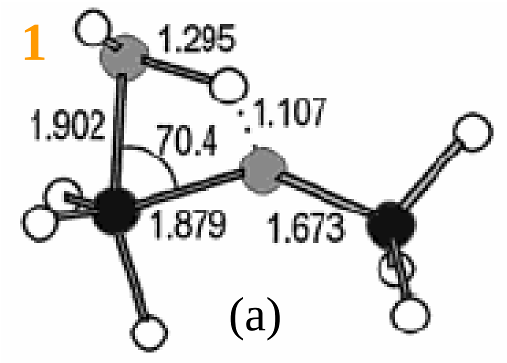


- ✓ The molecule has at least one lone (nonbonding) electron pair (Lewis base)
- ✓ The molecule possesses a labile proton (Bronsted acid)
- ✓ The distance between the acid and base sites conforms with the Si-O bond distance

T. A. Michalske and B. C. Bunker, J. Appl. Phys. 56 (10) (1984) 2686-2693

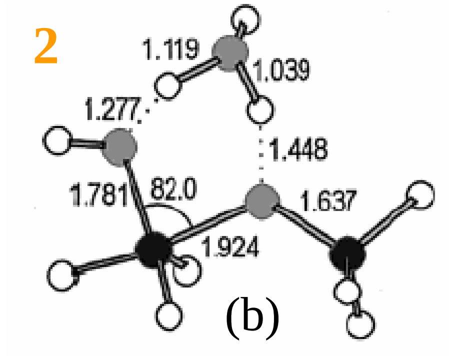
Multiple Water Molecules Effect





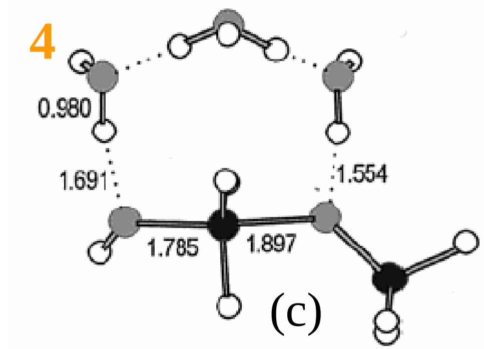
Transition state for disiloxane with one water molecule

ΔEa = 33.9 kcal/mol



Transition state for disiloxane with two water molecules

ΔEa = 24.7 kcal/mol



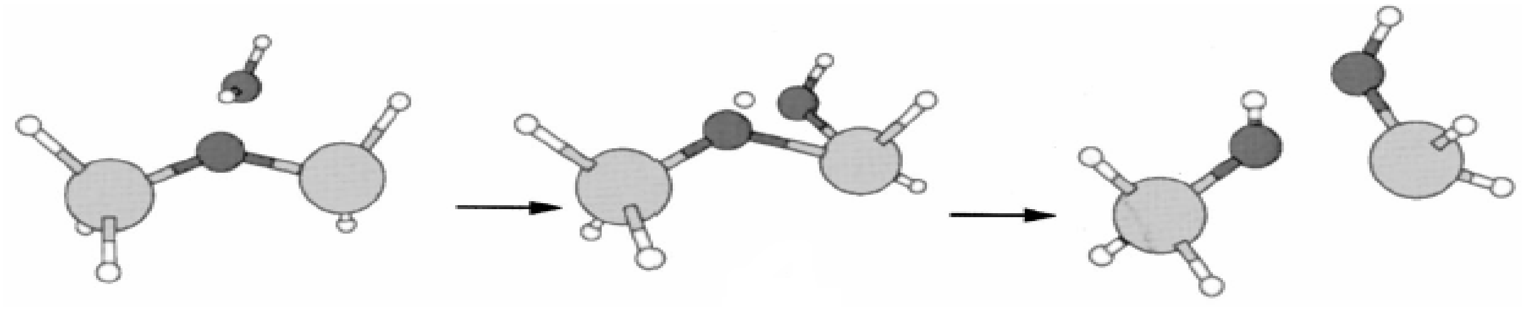
Transition state for disiloxane with four water molecules

ΔEa = 23.0 kcal/mol

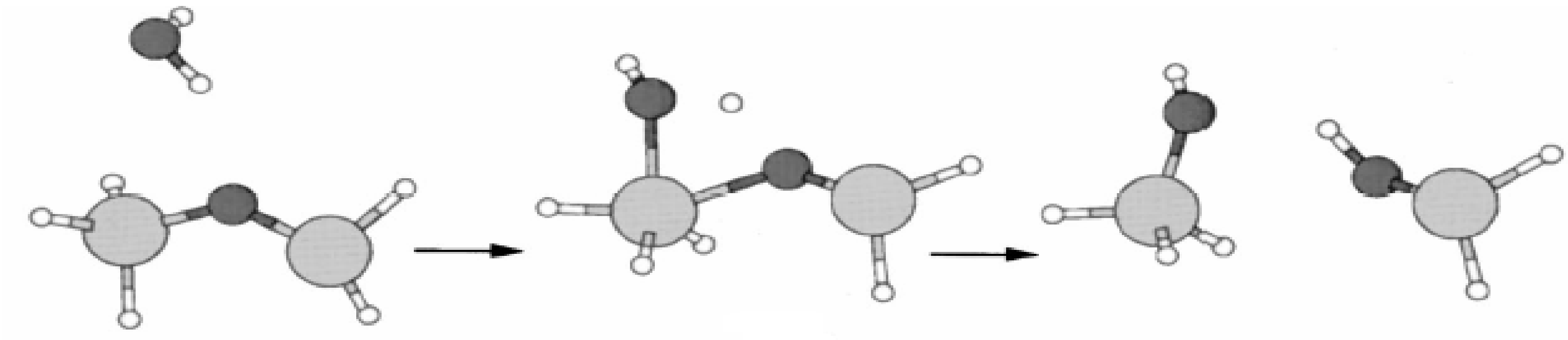
Decreasing activation energy with increasing numbers of water molecule

Marek Cypryk and Yitzhak Apeloig, Organometalics 2002, 21, 2165-2175

Surface Defect (dangling bond) Effect



ΔEa = 96.0 kJ/mol by using UB3-LYP/6-31G*



ΔEa = 120.8 kcal/mol by using UB3-LYP/6-31G*

Lower activation energy for reaction around defect site

Tiffany R. Walsh, Mark Wilson, and Adrian P. Sutton, J. Chem. Phys. Vol. 113, No. 20, 9191-9201 (2000)

Conclusion

- ✓ **The subcritical crack curve is composed of three regions, reaction-controlled region, transport-controlled region, and catastrophic failure.**
- ✓ **The presence of water vapor increased crack velocity. The threshold energy release rate changes linearly with the logarithm of water pressure.**
- ✓ **Crack velocity increased with increasing concentration of hydroxyl ion. Threshold energy release rate changes linearly with PH.**
- ✓ **Quantum chemistry calculation is promising the study of subcritical crack.**