PURDUE UNIVERSITY

NCN

www.nanohub.org

# ECE695: Reliability Physics of Nano-Transistors

## Lecture 11: Temperature dependence of NBTI

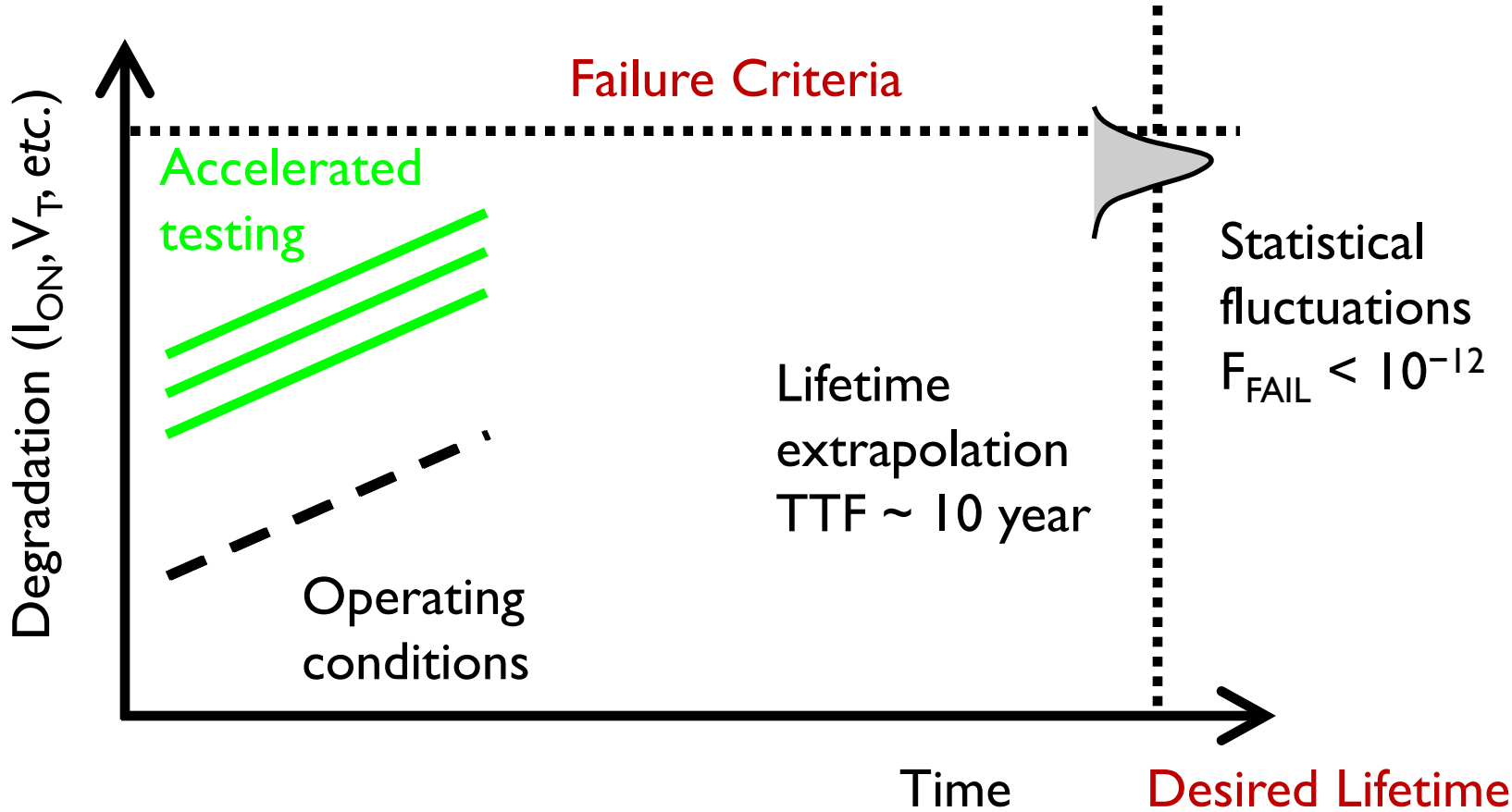
Muhammad Ashraful Alam
alam@purdue.edu

# Copyright 2013

# Outline

1. Review: Temperature activation & NBTI
2. Temperature dependent forward/reverse rates
3. Temperature dependence of diffusion coefficient
4. Material dependence of activation energy
5. Conclusion

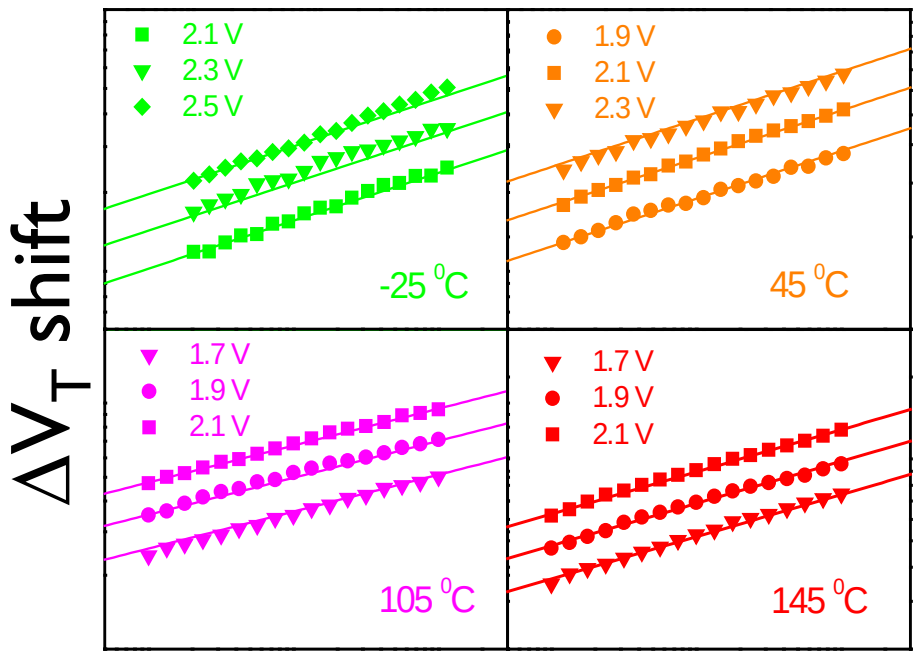
# Importance of Voltage/Temperature Acceleration



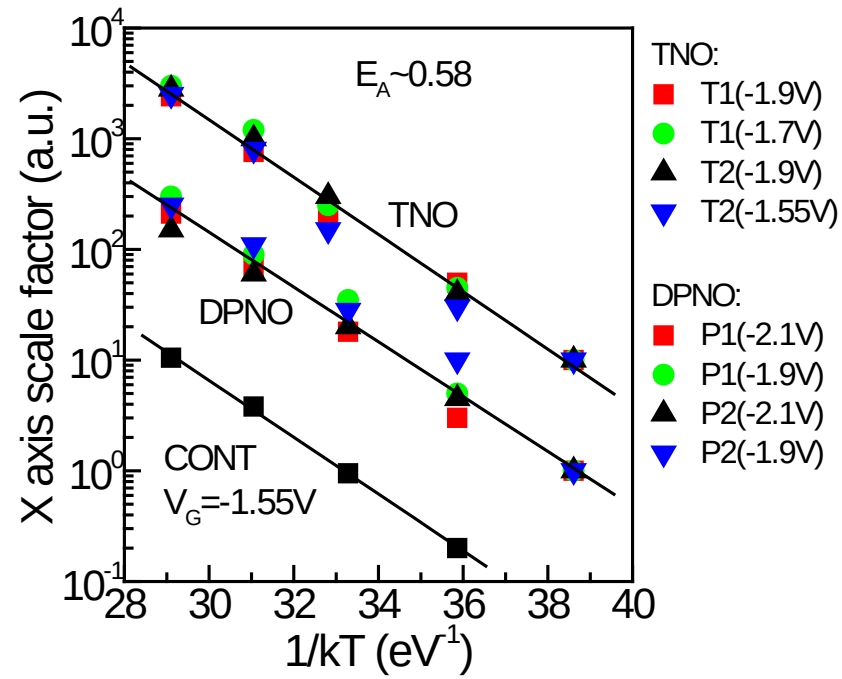

$V_G, V_D, V_B, T$ → DUT → Reliability Predictions

# Field and temperature dependencies

$$\Delta V_T = A(E) \times e^{-E_A/nk_BT} \times g(f,d) \times t^n$$




Stress time

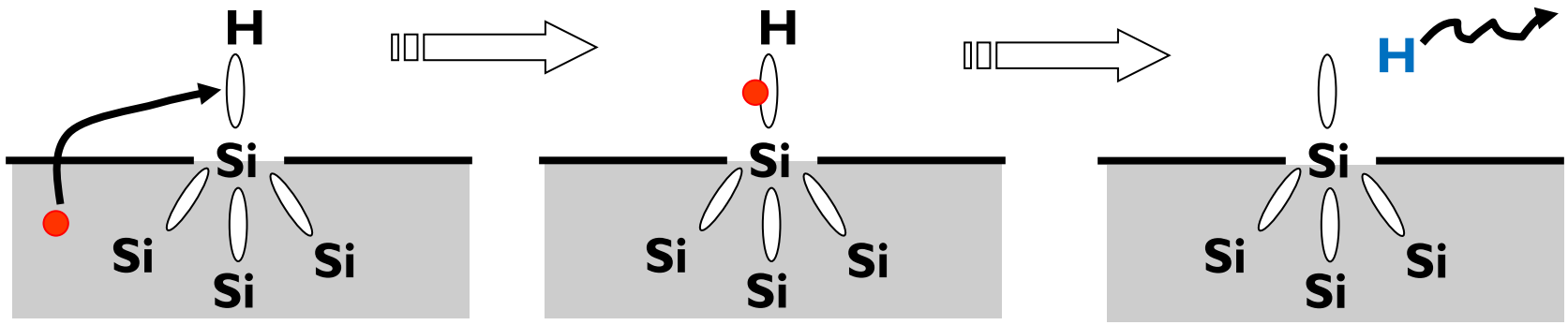


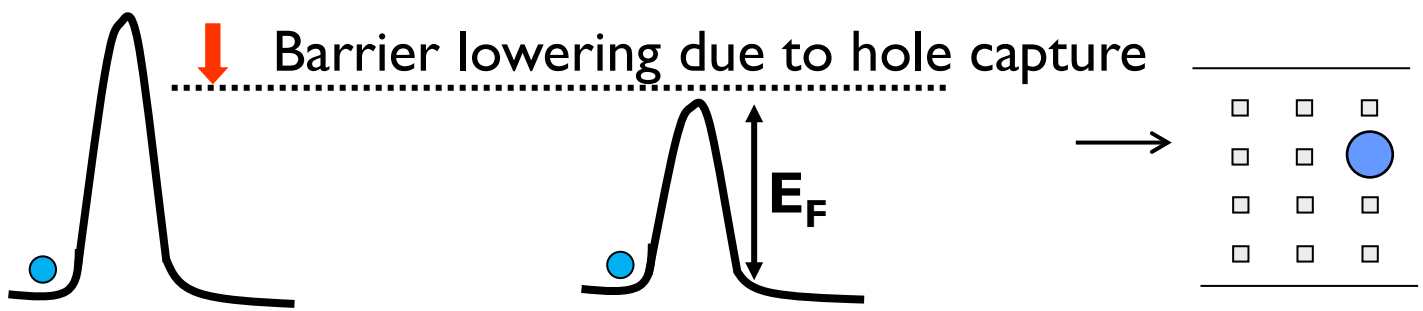

$E_A$~0.58 eV

# Temperature dependence of NBTI

$T_H \sim \exp(\gamma_T . E_{OX})$

$p_H \sim E_C$




Hole capture  Bond dissociation  H-diffusion

# Interface traps with $H_2$ diffusion

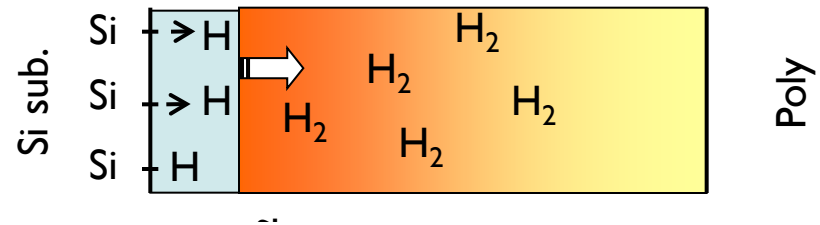
$$\left(\frac{k_F N_0}{k_R}\right) \approx N_H(0) N_{IT}$$

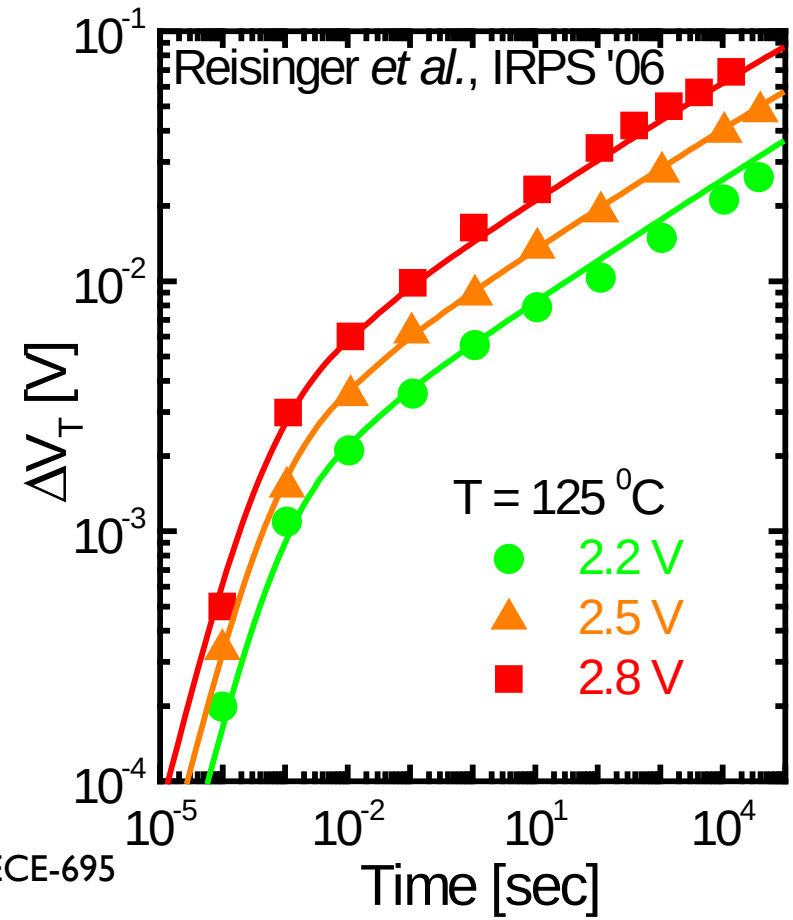
$$N_{IT}(t) = \frac{1}{2} N_{H_2}(0)\sqrt{D_{H_2} t}$$

$$const. = \frac{N_H(0)^2}{N_{H_2}(0)} \quad (2H \square \quad H_2)$$

**Combining the three, we get**

$$N_{IT}(t) \propto \left(\frac{k_F N_0}{2k_R}\right)^{2/3} (D_{H_2} t)^{1/6}$$



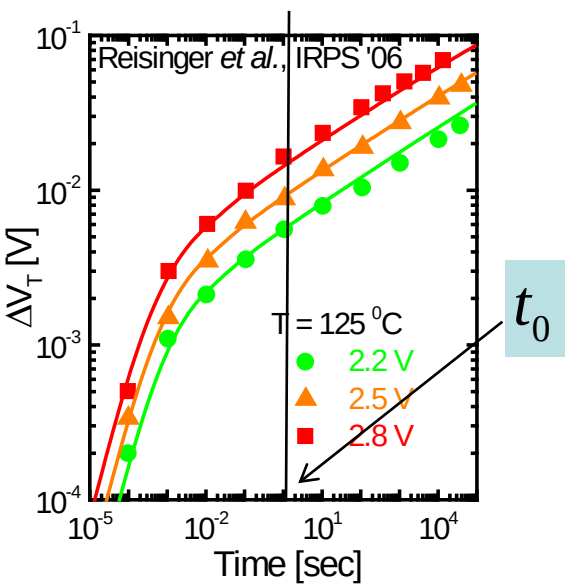
# How to determine the temperature activation?

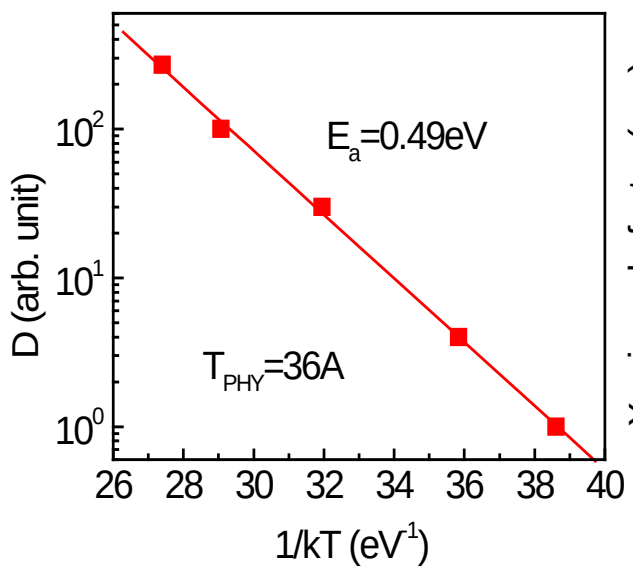
$$N_{IT} = \left(\frac{k_F N_0}{k_R}\right)^m (D_H t)^n \qquad k_F = k_{F0} \times e^{-\frac{E_F}{k_B T}} \qquad k_R = k_{R0} \times e^{-\frac{E_R}{k_B T}} \qquad D_H = D_{H0} e^{-\frac{E_H}{k_B T}}$$

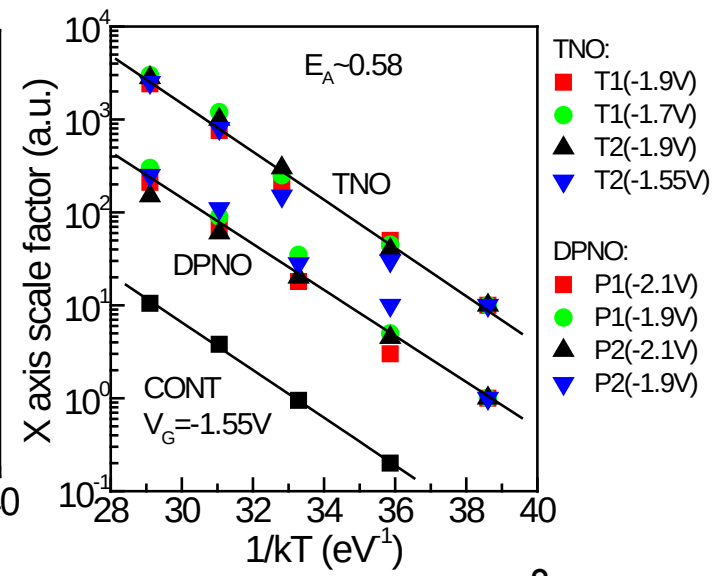
$$= \left(\frac{k_{F0} N_0}{k_{R0}}\right)^m \left[D_{H0} e^{-\left\{m\frac{E_F - E_R}{n} + E_H\right\}/k_B T}\right]^n \times \left[t^n\right]$$

$$\ln(N_{IT}(T, t_0) = \ln A(t_0) - E_A / k_B T$$

$$E_A = m\frac{(E_F - E_R)}{n} + E_H$$



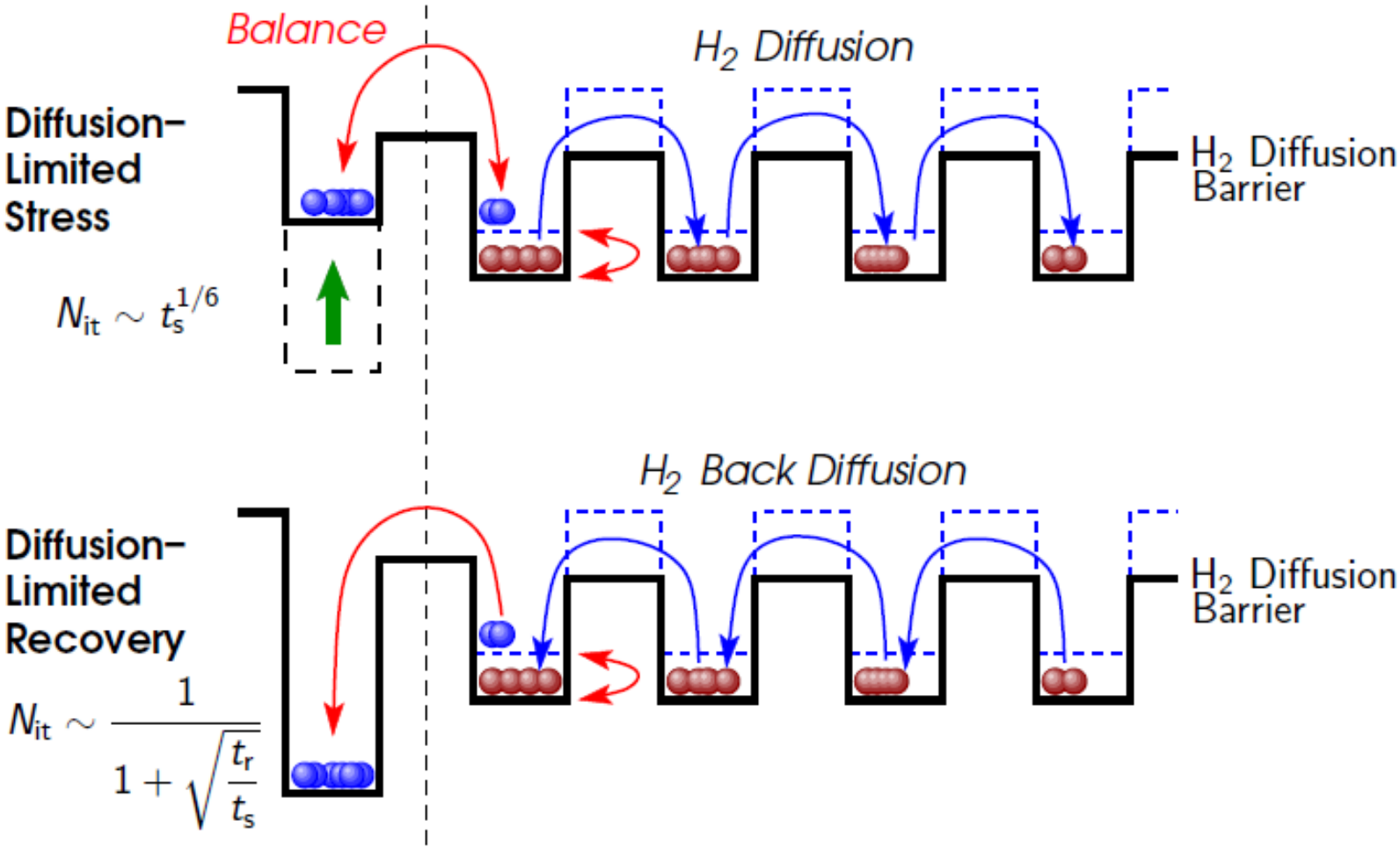



# Outline

1. Review: Temperature activation & NBTI
2. Temperature dependent forward/reverse rates
3. Temperature dependence of diffusion coefficient
4. Material dependence of activation energy
5. Conclusion

# Temperature dissociation of Si-H bonds



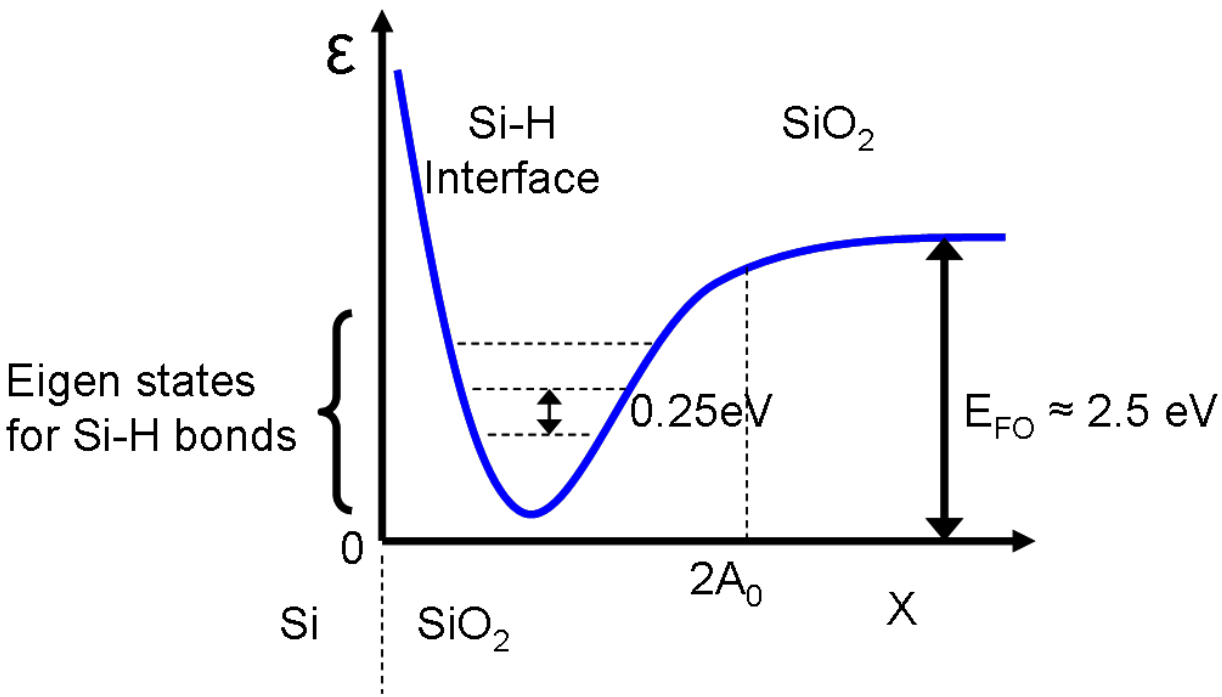

*Taken from T. Grasser, IRPS Tutorial, 2007.*

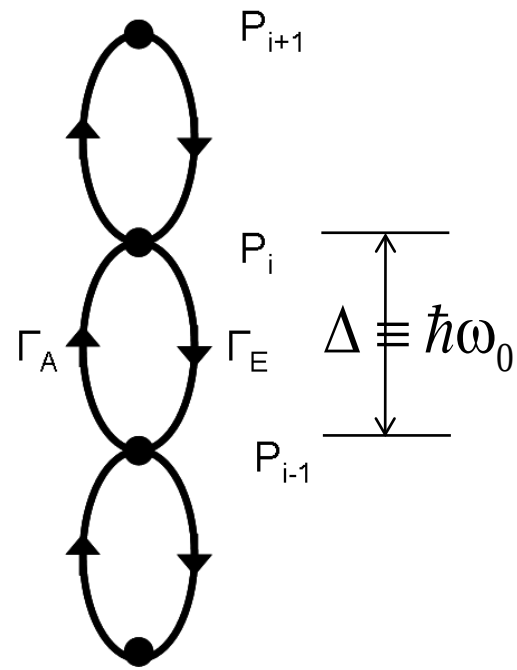
# T-dependence of $k_F$ and $k_R$

Derive … $k_F = k_{F0} \times e^{-\frac{E_F}{k_B T}} \propto (n_{max} + 1) \times e^{-\frac{E_F}{k_B T}}$

$$k_F = \Gamma_0 \left(n_{max} + 1\right) \times \Gamma_E \left[\frac{\Gamma_A}{\Gamma_E}\right]^{n_{max}+1} \qquad n_{max} \equiv \frac{E_F}{\hbar\omega_0} = \frac{E_F}{\Delta}$$

Consider an harmonic oscillator with equally spaced levels …



# Transition rates due to phonons

In a harmonic oscillator …

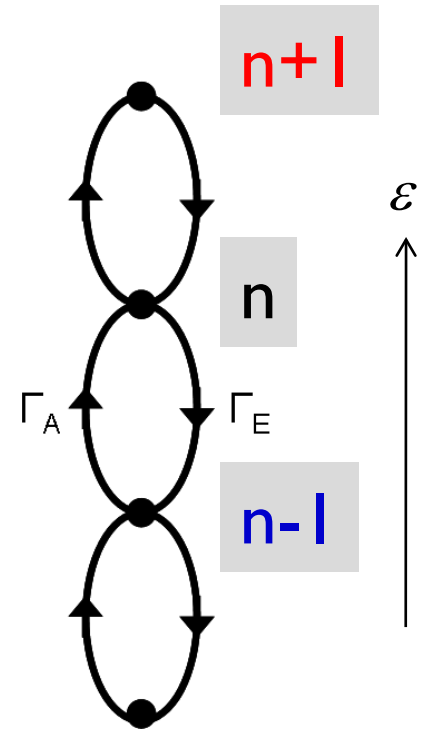
$$Au_n = \sqrt{n}\, u_{n-1}$$

$$\langle n-1 | A | n \rangle = \sqrt{n}\, \hbar$$

Therefore the transition rate is …

$$M_{(n-1)\to n} \equiv \frac{2\pi}{\hbar} \left| \langle n-1 | A | n \rangle \right|^2 = n\, h$$

$$F_{(n-1)\to n} \equiv nh \times \Gamma_A \times P_{n-1}$$




*Ref. Datta, Atom to Transistor, Cambridge, 2005.*

# Absorbing/Emitting phonons in Equilibrium

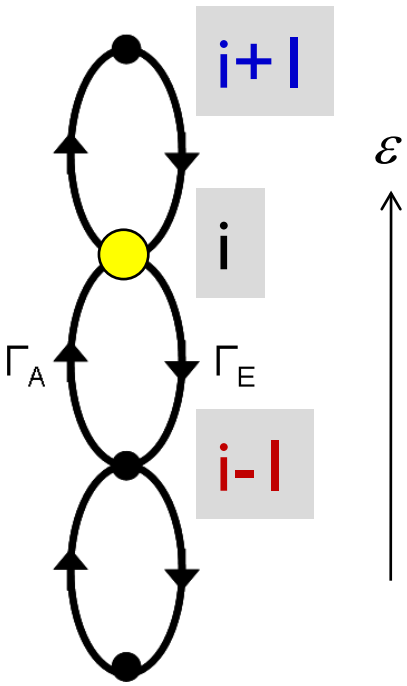
Probability of a Si-H bond at the i-th vibration mode …

$$i\Gamma_A P_{i-1} + (i+1)\Gamma_E P_{i+1} - (i+1)\Gamma_A P_i - i\Gamma_E P_i = 0$$

$$\Gamma_A = \Gamma_0\left(1 - \delta/2\right) \qquad \Gamma_E = \Gamma_O\left(1 + \delta/2\right) \qquad \frac{i+1}{i} \to 1$$

$$\left.\frac{d^2P}{d\varepsilon^2}\right]_i = \frac{P_{i-1} - 2P_i + P_{i+1}}{\Delta^2} = -\frac{\delta}{\Delta}\frac{2P_{i+1} - P_{i-1}}{2\Delta}$$

$$\frac{d^2P}{d\varepsilon^2} + \frac{\delta}{\Delta}\frac{dP}{d\varepsilon} = 0 \qquad \Rightarrow P(\varepsilon) = C \times e^{-\delta \times \varepsilon/\Delta}$$



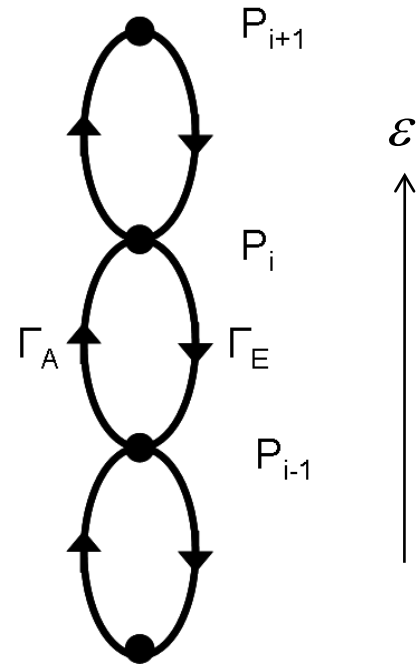

Does it remind you of BFWF Distribution in Lecture 3?!

# Absorbing/Emitting phonons in Equilibrium

$$P(\varepsilon) = C \times e^{-\delta \times \varepsilon / \Delta}$$

Detailed balance …

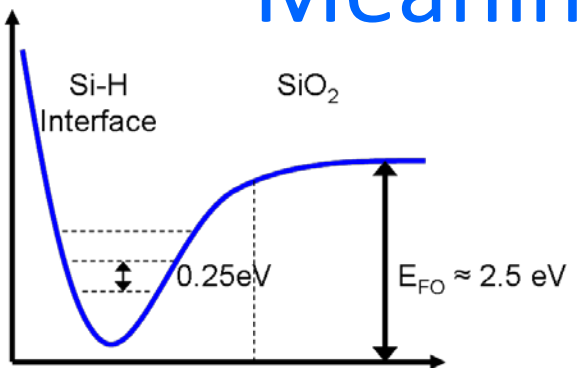
$$\left.\begin{aligned} \frac{\Gamma_A}{\Gamma_E} &= e^{-\Delta/k_B T} \approx 1 - \frac{\Delta}{k_B T} \\ \frac{\Gamma_A}{\Gamma_E} &= \frac{\Gamma_0 (1-\delta/2)}{\Gamma_0 (1+\delta/2)} = 1-\delta \end{aligned}\right\} \quad \delta = \frac{\Delta}{k_B T}$$

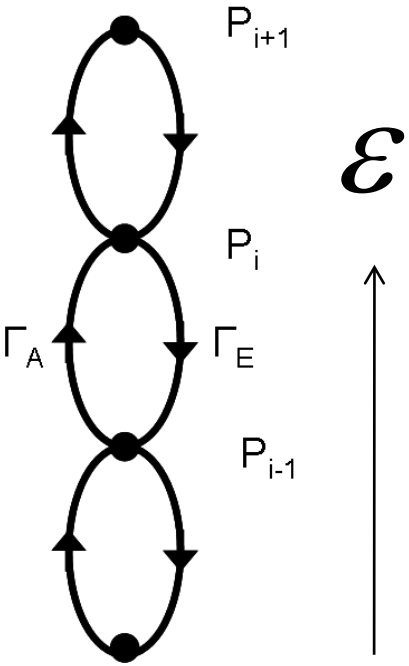


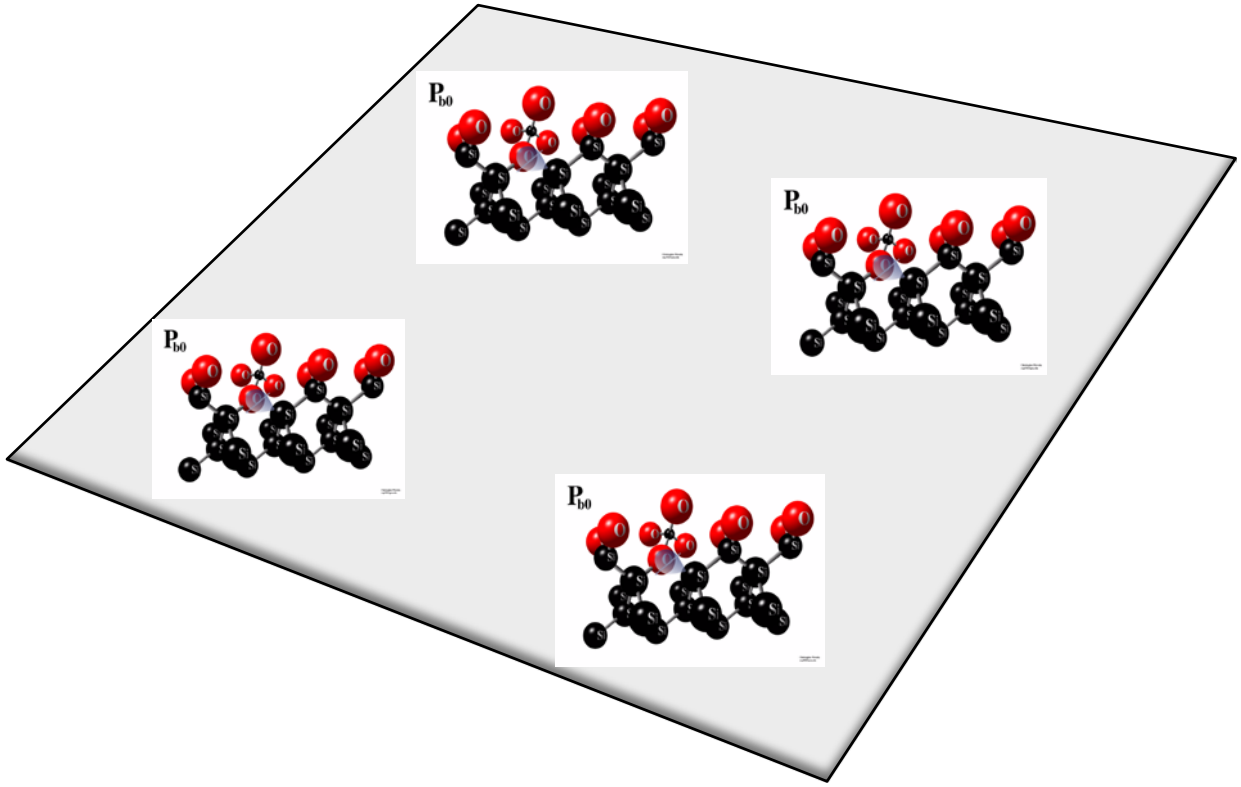

$$P(\varepsilon_i) = C \times e^{-\varepsilon_i / k_B T}$$ and C by normalization $$\sum_i p(\varepsilon_i) = 1$$

Approximate Bose-Einstein distribution

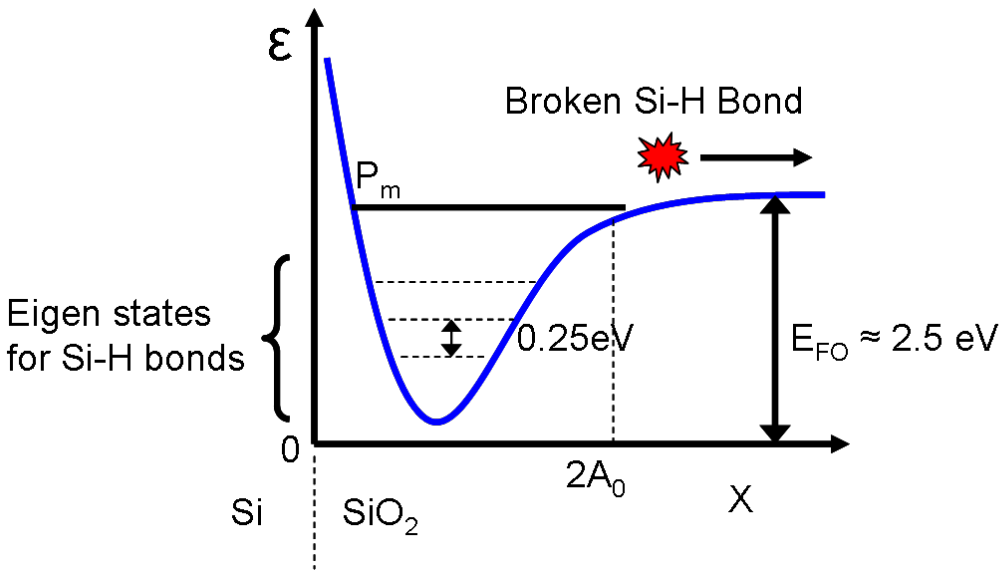
# Meaning of the distribution …

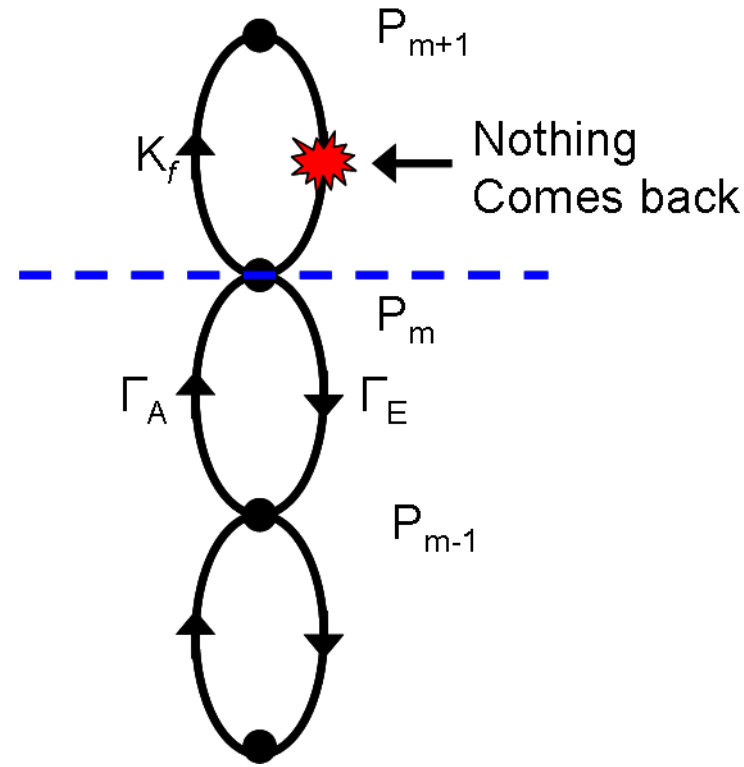


# Non-equilibrium dissociation of Si-H bonds




$$k_F = (n_{\max}+1)\times\Gamma_A P_n = (n_{\max}+1)\times\Gamma_E P_{n+1}$$

$$= (n_{\max}+1)\times\Gamma_A \times e^{-(n_{\max}+1)\Delta/k_B T}$$

$$k_F = (n_{\max}+1)\Gamma_E\left[e^{-\Delta/k_B T}\right]^{(n_{\max}+1)}$$

$$= (n_{\max}+1)\times\Gamma_E\left[\Gamma_A/\Gamma_E\right]^{n_{\max}+1} = (n_{\max}+1)\times\Gamma_A\left[\Gamma_A/\Gamma_E\right]^{n_{\max}} = (n_{\max}+1)\times\Gamma_A e^{-\frac{E_F}{k_B T}}$$

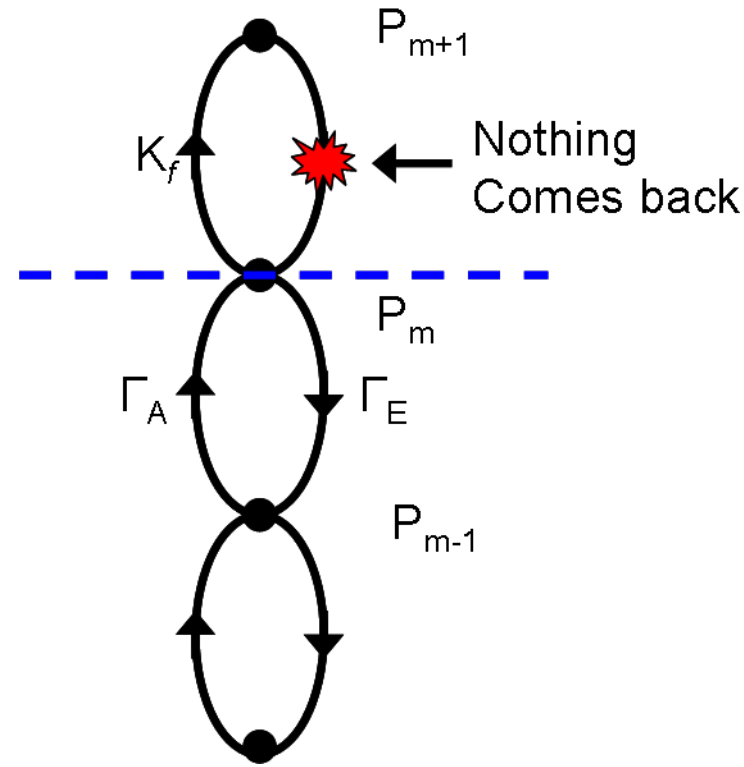
# Interpretation

Probability that a Si-H climbs the barrier

… that it finally absorbs a phonon to break the bond

$$k_F = (n_{\max} + 1) \times \Gamma_A \times e^{-\frac{E_F}{k_B T}}$$

$$\equiv k_{F0} \times e^{-\frac{E_{F0}}{k_B T}}$$

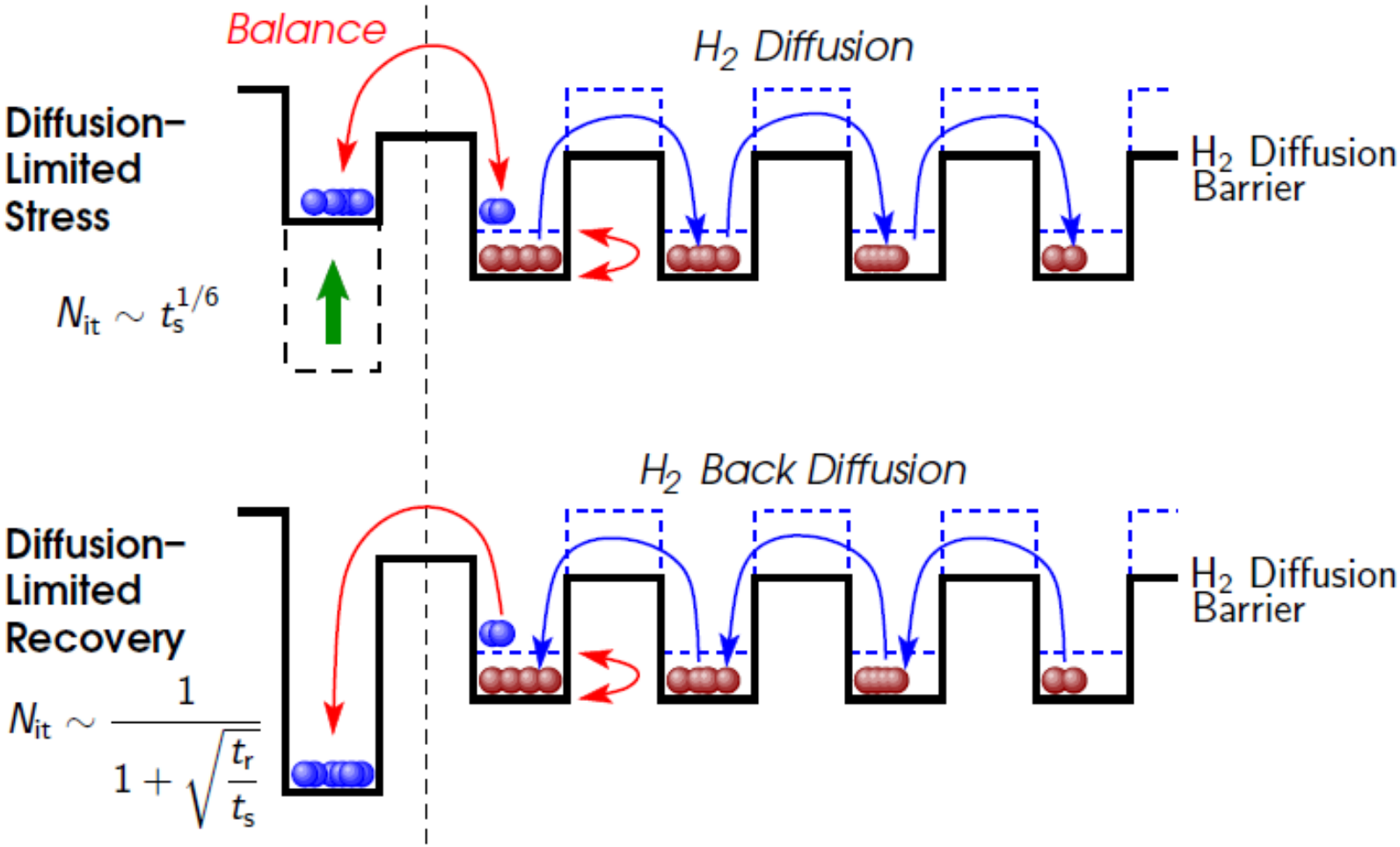



See Appendix A for full derivation

# Outline

1. Review: Temperature activation & NBTI
2. Temperature dependent forward/reverse rates
3. Temperature dependence of diffusion coefficient
4. Material dependence of activation energy
5. Conclusion

# Temperature dissociation of Si-H bonds

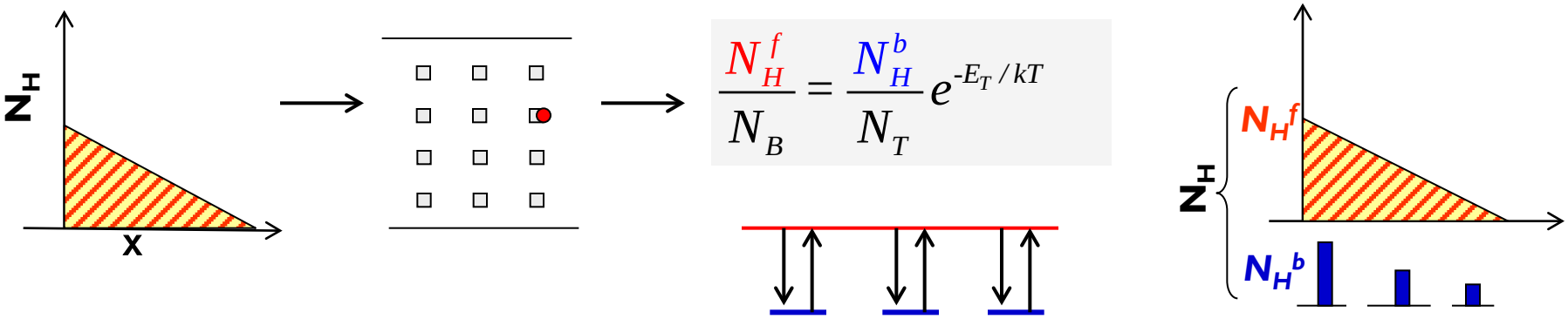



*Taken from T. Grasser, IRPS Tutorial, 2007.*

# Origin of activated diffusion

$$D_H = D_0\, e^{-E_H/k_B T}$$

Standard Distribution | Real-Space | Energy-Space | Real Distribution



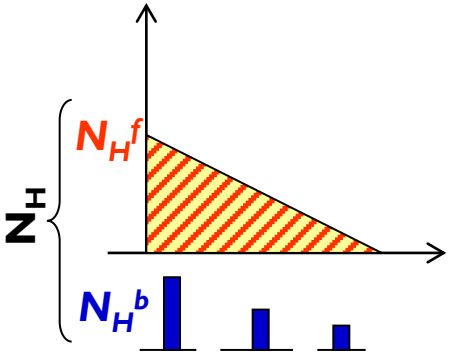

$$\frac{N_H^f}{N_B} = \frac{N_H^b}{N_T} e^{-E_T/kT}$$

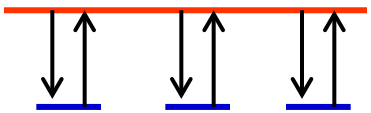
$$\frac{dN_{IT}}{dt} = D_0^* \frac{d^2 N_H^f}{dx^2}$$

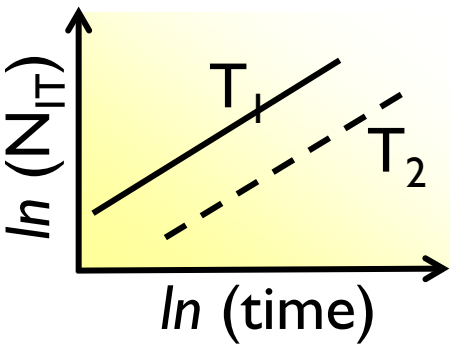
$$\frac{dN_H^f}{dt} = -\frac{N_H^f / N_c}{\tau_c} + \frac{N_H^b / N_T}{\tau_e}$$

$$N_H^f \approx \left(\frac{N_c}{N_T}\right) N_H^b \left(\frac{\tau_c}{\tau_e}\right) \sim \left(\frac{N_c}{N_T}\right) N_H^b\, e^{-\frac{E_H}{k_B T}}$$

# Activated diffusion: A counting trick!






$$\frac{dN_{IT}}{dt} = D_0^* \frac{d^2 N_H^f}{dx^2} \Rightarrow N_H^f \sim \left( \frac{N_B}{N_T} e^{-E_T/k_B T} \right) N_H \Rightarrow \frac{dN_{IT}}{dt} = D_H \frac{d^2 N_H}{dx^2}$$

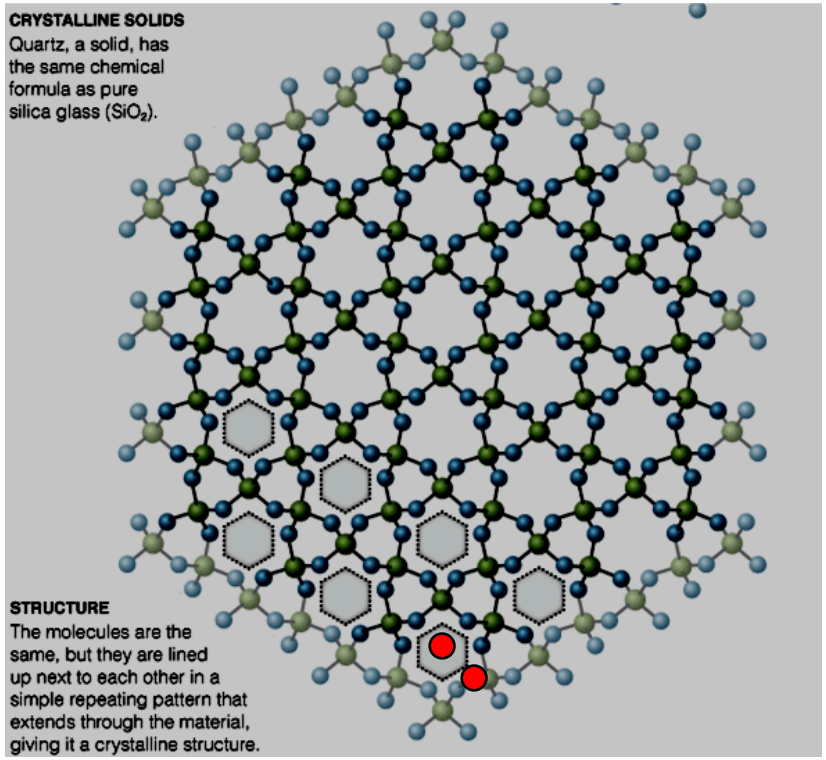
$$D_0^* = a^2 v_0$$

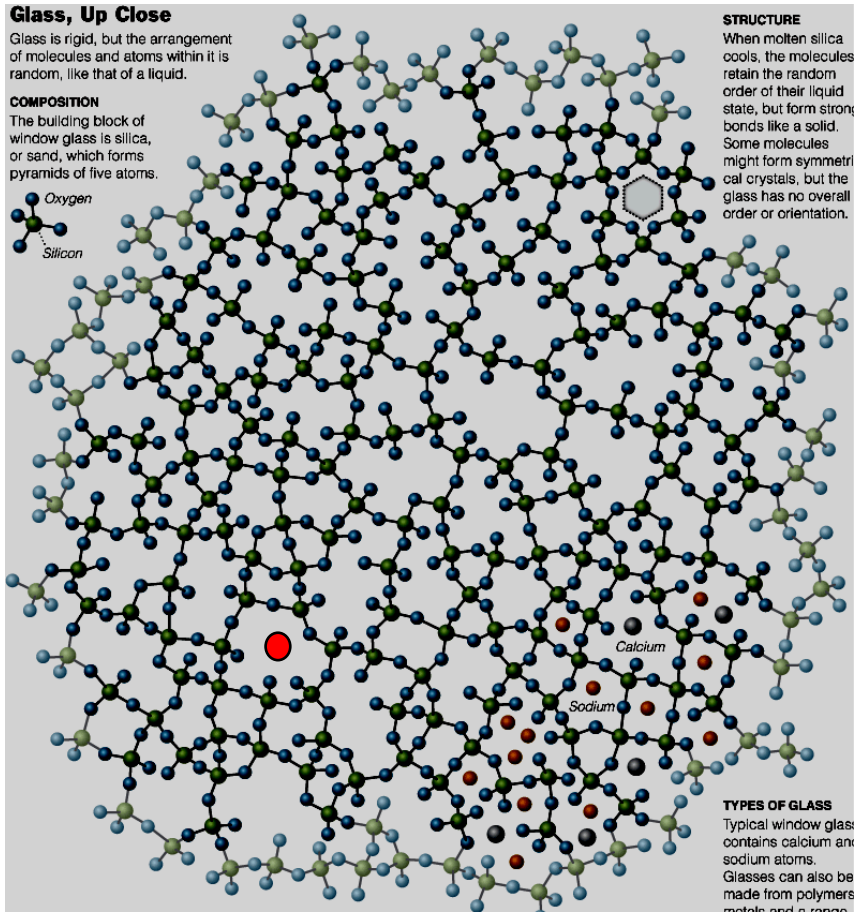
$$\frac{N_H^f}{N_B} = \frac{N_H^b}{N_T} e^{-E_T/kT}$$

$$D_H = D_0^* \frac{N_B}{N_T} e^{-Ea/kT} \equiv D_0 e^{-Ea/k_B T}$$

Ratio of free vs. trapped H determines properties of diffusion coefficient

# Crystalline vs. Amorphous Oxides



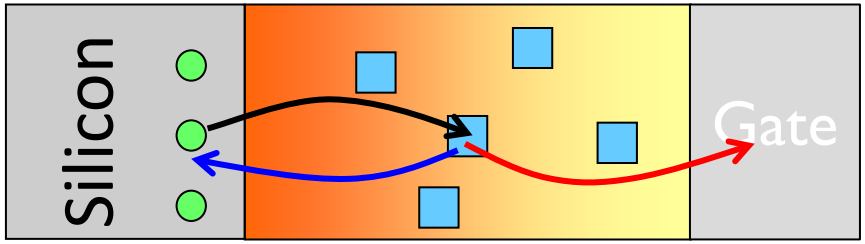

**'Glass up Close',**

*NY Times, July 29, 2008.*

# Outline

1. Review: Temperature activation & NBTI
2. Temperature dependent forward/reverse rates
3. Temperature dependence of diffusion coefficient
4. Material dependence of activation energy
5. Conclusion

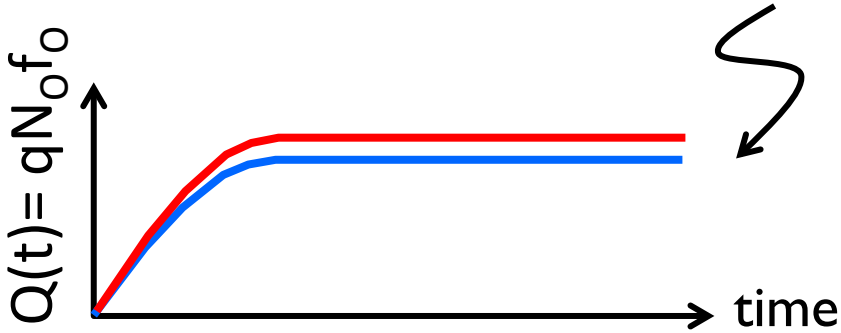
# Voltage-shift due to pre-existing traps in thin oxides




$$f_O \equiv \frac{n}{N_O}$$

$$\frac{dn_O}{dt} = \frac{d(N_O f_O)}{dt} = N_O \sigma \upsilon_{th}\left[n_e T_1 (1 - f_O) - p_S T_1 f_O - p_G T_2 f_O\right]$$

$$f_O = \frac{T_1\left[1-\exp\left(-\sigma\upsilon_{th}\left(n_e T_1 + p_s T_1 + p_G T_2\right)t\right)\right]}{\left(1+p_S/n_e\right)T_1 + p_G T_2/n_e} \equiv b(T)\left[1-\exp\left(-t/\tau_c(T)\right)\right]$$

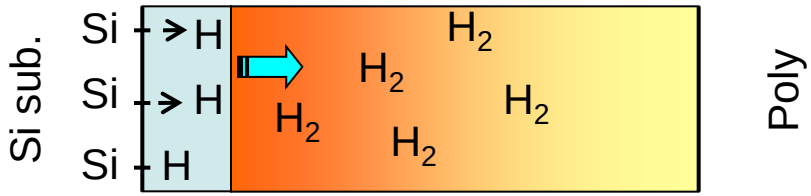


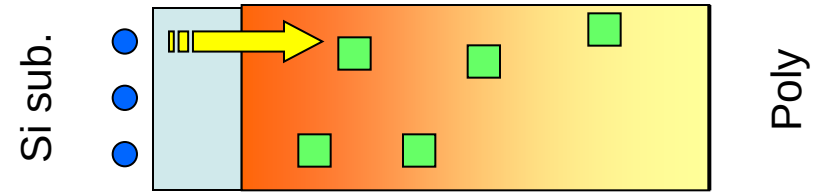

$$\tau_c \propto T_1^{-1} \propto e^{+\frac{x}{x_0}}$$

$$n_e = C_O\left(V_G - V_T(T)\right) \Rightarrow \Delta n_e = -C_O \Delta V_T(T) \propto k_B T$$

Weak T-dependence

# Temperature activation (with Hole trapping)




$$\Delta V_T(T,t) \square \Delta V_H(T,t) + \Delta V_{IT}(T,t)$$

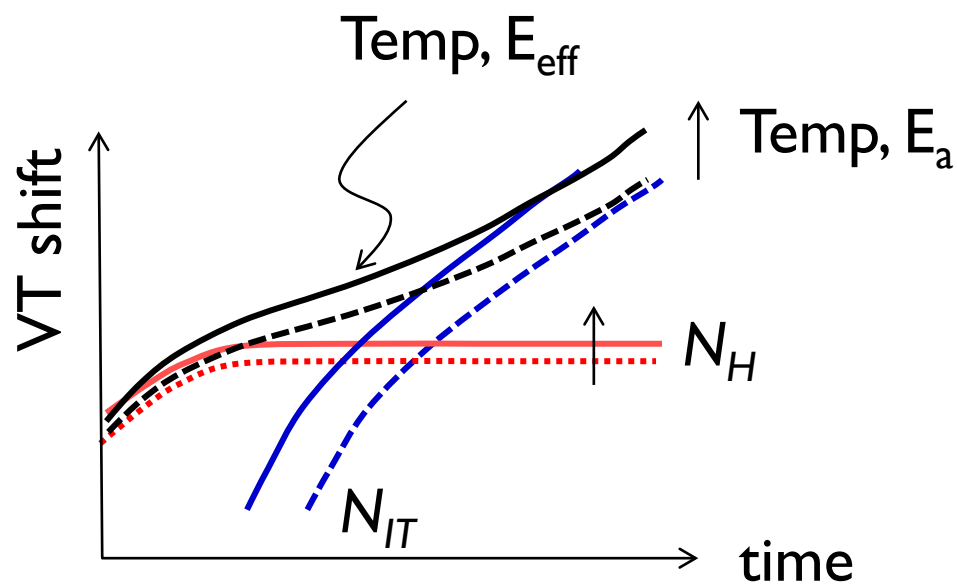
$$= A \times (k_B T) + B e^{-E_a/k_B T} t^n$$

Effective activation energy

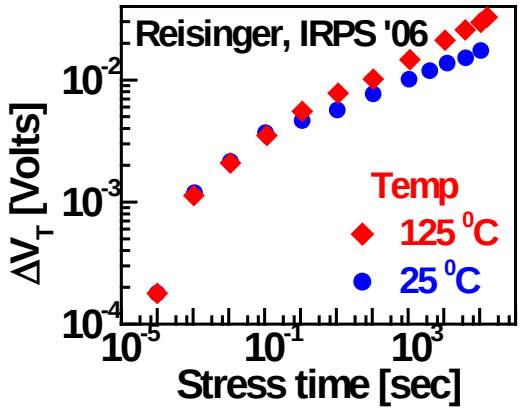
$$ln\left[\Delta V_T(T,t_0)\right]$$

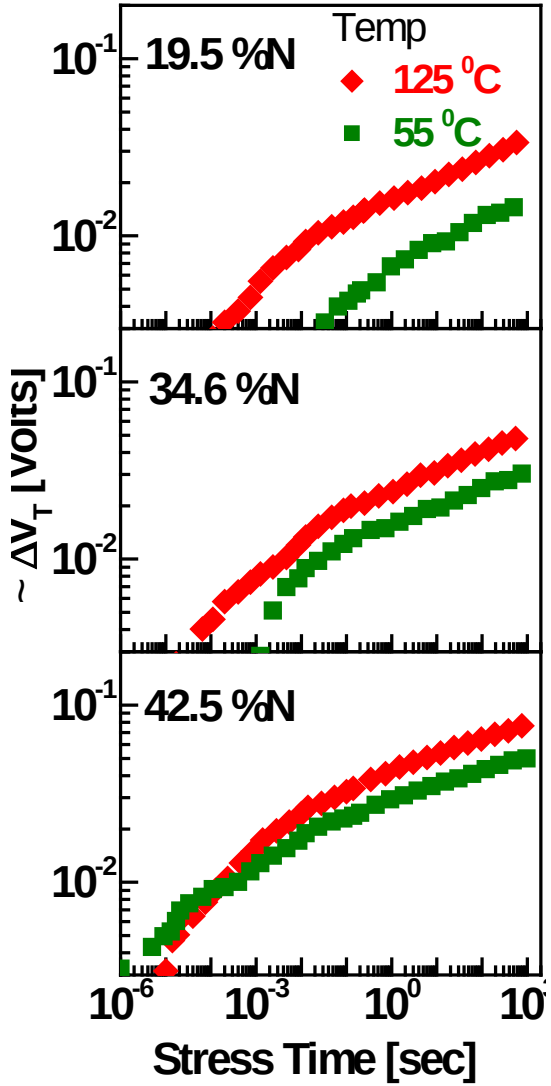
$$= ln\left[A \times k_B T + B e^{-E_a/k_B T} t_0{}^n\right]$$

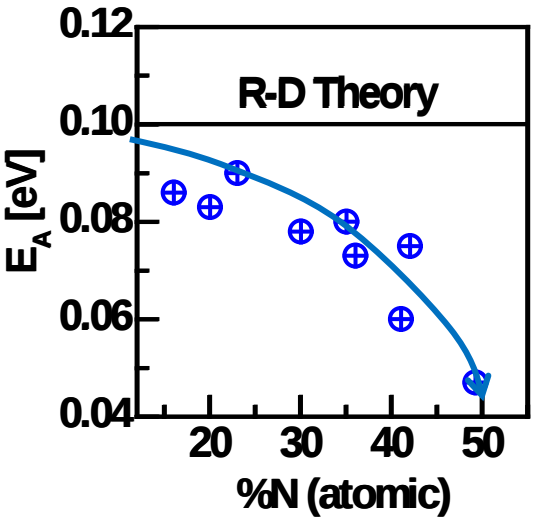
$$= ln\left[C e^{-E_{eff}/k_B T}\right]$$



# Nitrogen increases hole trapping and reduces effective EA

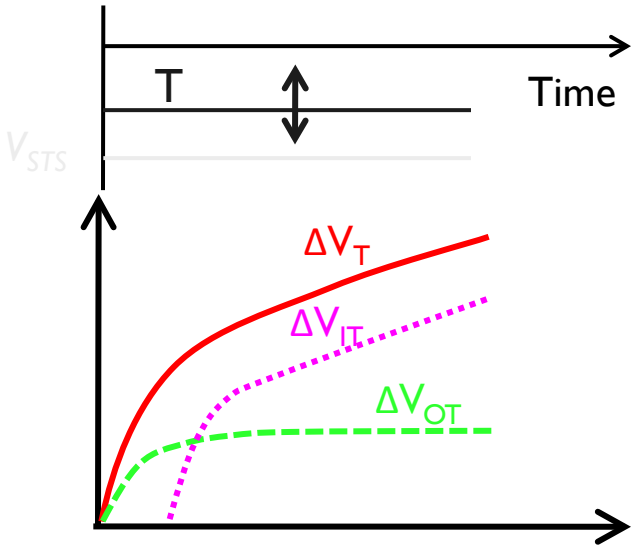


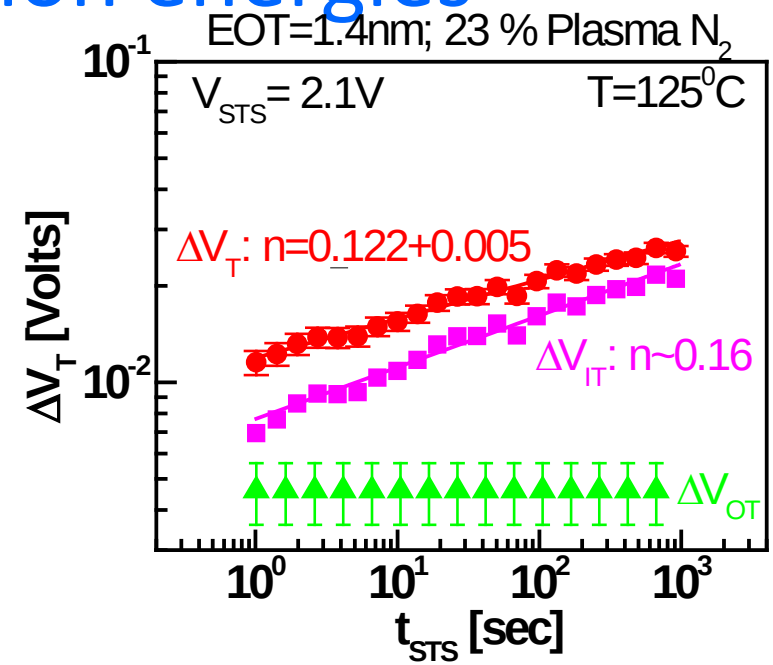



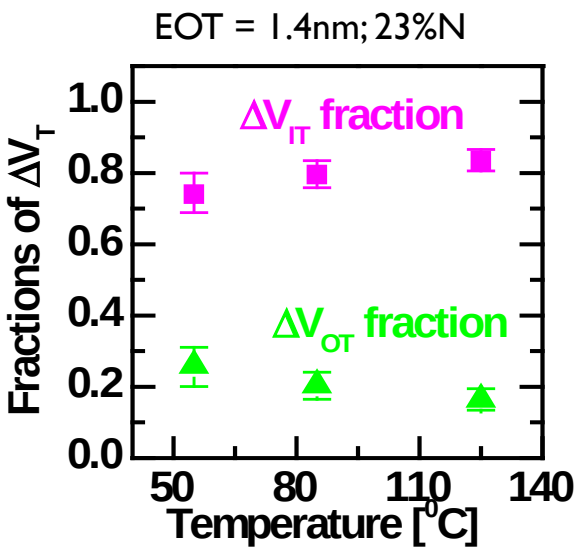



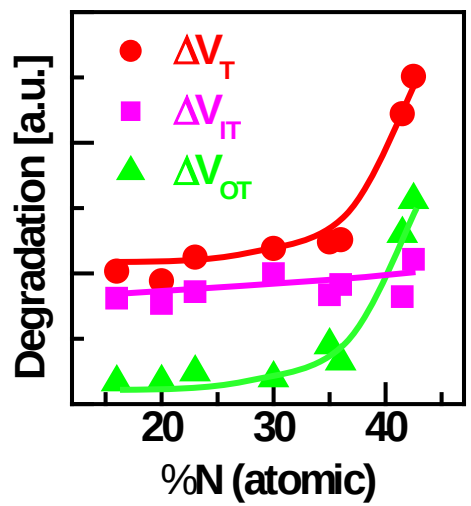

- %N reduces T dependence
- Effect more visible in short $t_{STS}$

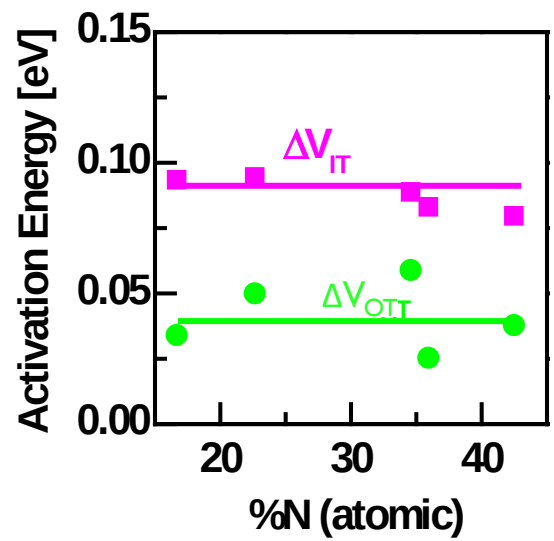
# $N_{IT}/N_{OT}$ decomposition & calculation of activation energies



# Conclusion

- We have discussed the origin of temperature dependent activation of the dissociation rates and the diffusion coefficients.

- There is an important distinction between thermally activated vs. electrically stimulated breaking of bonds. This distinction is important for understanding NBTI and HCI degradation.

- Activated diffusion implies subpopulations that are mobile that can rapidly exchange positions with 'bound' or 'trapped' subpopulation. In this sense, it is very different from classical thermal diffusion of electrons/holes.

# References


- For diffusion in complex media, see Fractional Kinetics, I. Sokolov, J. Klafter, and A. Blumen, Physics Today, Nov. 2002, page. 48.
- .The detailed theory of relative contribution of hole trapping and SiH bond dissociation is discussed in "A Critical reevalution of RD model for NBTI stress and recovery" by S. Mahapatra, IRPS Proc. 2011

# Self-Test Questions

- Does Einstein relationship hold for activated diffusion?
- People argue that the forward dissociation and reverse passivation have similar activation barriers. Would you support the argument?
- What assumption did I make regarding diffusion of H in SiO2 that makes the derivation slightly imprecise? Hint. Crystal vs. amorphous structure.
- Can you explain physically why tunneling is less temperature sensitive than SiH bond dissociation?
- Would the "observed activation energy" decrease or increase if there are significant hole trapping?
- Where does the entropy hide in classical rate equations? How do we account for it when we discuss semiconductor physics?

PURDUE UNIVERSITY

NCN

www.nanohub.org

# ECE695: Reliability Physics of Nano-Transistors

## Lecture 11: Appendices

## Temperature dependence of NBTI

Muhammad Ashraful Alam
alam@purdue.edu

# Appendices

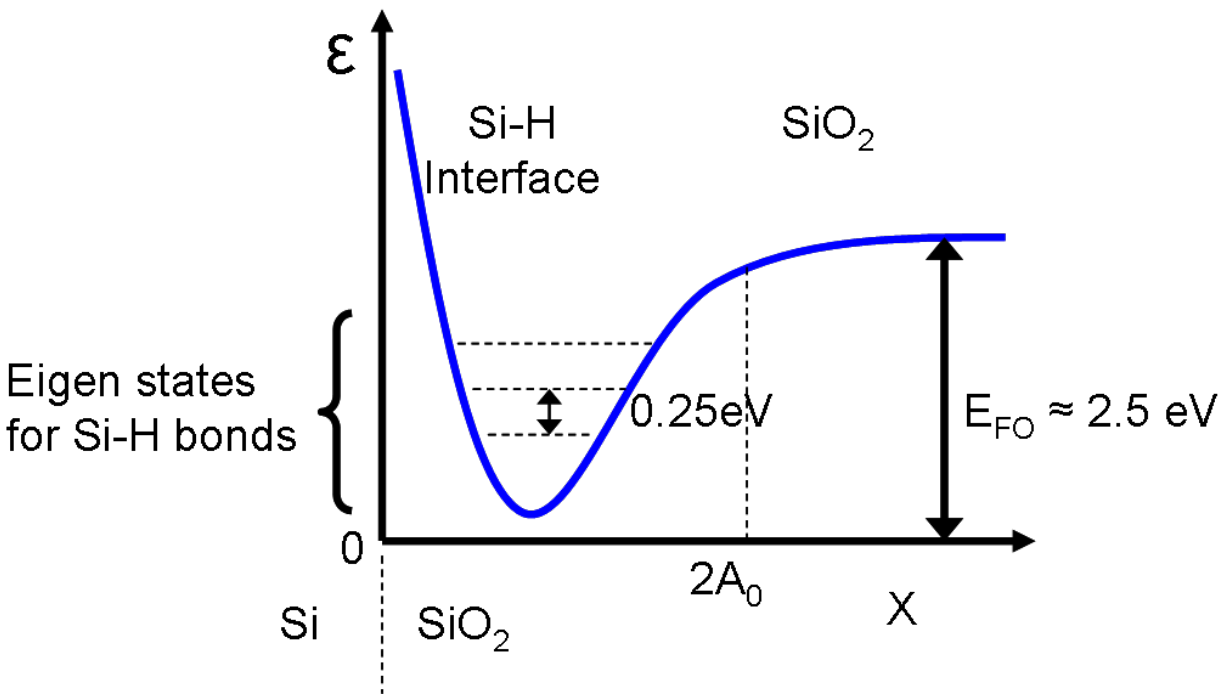
1. Derivation of forward and reverse dissociation
2. Bose Einstein vs. Boltzmann distribution
3. Theory of Dispersive diffusion
4. Conclusion

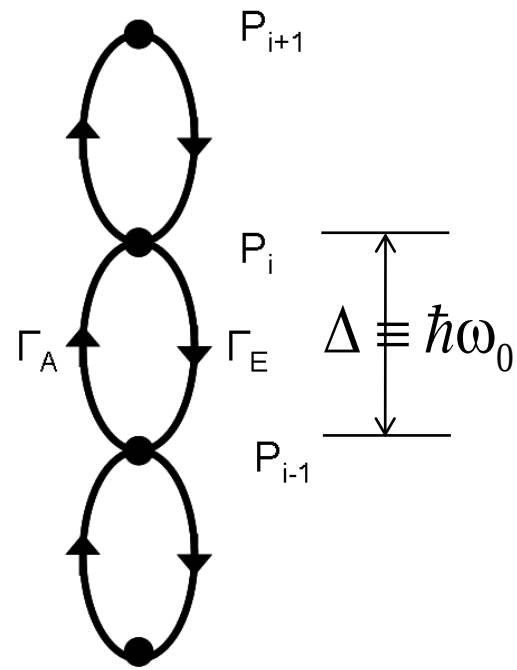
# Appendix 1: T-dependence of $k_F$ and $k_R$

Derive … $k_F = k_{F0} \times e^{-\frac{E_F}{k_B T}} \propto (n_{max}+1) \times e^{-\frac{E_F}{k_B T}}$

$$F = \Gamma_0 \left(n_{max}+1\right) \times \left[\frac{\Gamma_{ext}}{\Gamma_{ext}+\Gamma_0}\right]^{n_{max}+1} \qquad n_{max} \equiv \frac{E_F}{\hbar\omega_0} = \frac{E_F}{\Delta}$$

Consider an harmonic oscillator with equally spaced levels …



# Transition rates due to phonons

In a harmonic oscillator …

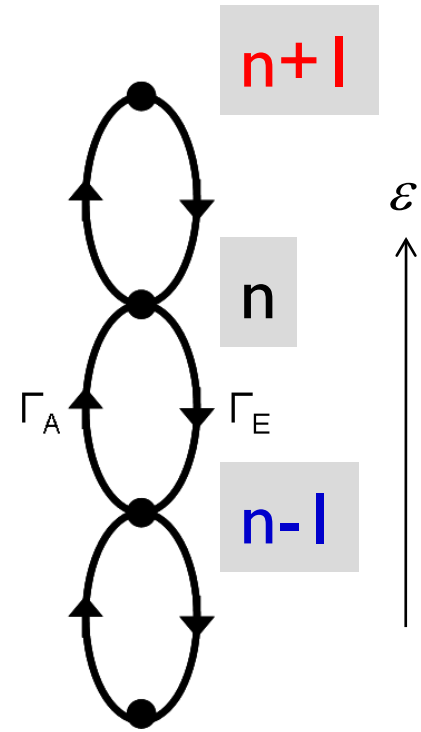
$$Au_n = \sqrt{n}\, u_{n-1}$$

$$\langle n-1 | A | n \rangle = \sqrt{n}\, \hbar$$

Therefore the transition rate is …

$$M_{n-1,n} \equiv \frac{2\pi}{\hbar} \left| \langle n-1 | A | n \rangle \right|^2 = n\, h$$

$$F_{(n-1)\to n} \equiv nh \times \Gamma_A \times P_{n-1}$$




*Ref. See Datta, Atom to Transistor, Cambridge, 2005.*

# Absorbing/Emitting phonons in Equilibrium

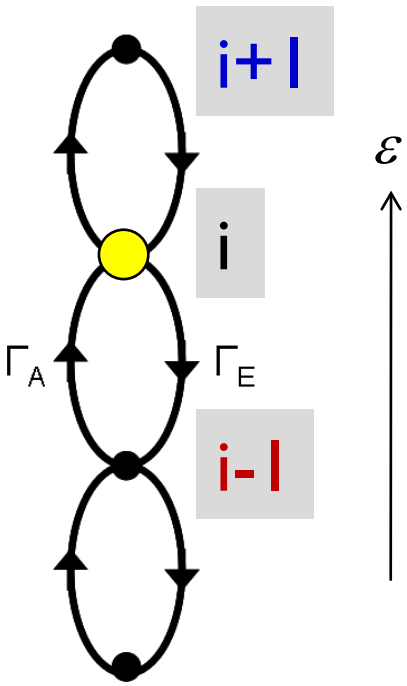
Probability of a Si-H bond at the i-th vibration mode …

$$i\Gamma_A P_{i-1} + (i+1)\Gamma_E P_{i+1} - (i+1)\Gamma_A P_i - i\Gamma_E P_i = 0$$

$$\Gamma_A = \Gamma_0\left(1 - \delta/2\right) \qquad \Gamma_E = \Gamma_O\left(1 + \delta/2\right) \qquad \frac{i+1}{i} \to 1$$

$$\left.\frac{d^2P}{d\varepsilon^2}\right]_i = \frac{P_{i-1} - 2P_i + P_{i+1}}{\Delta^2} = -\frac{\delta}{\Delta}\frac{2P_{i+1} - P_{i-1}}{2\Delta}$$

$$\frac{d^2P}{d\varepsilon^2} + \frac{\delta}{\Delta}\frac{dP}{d\varepsilon} = 0 \qquad \Rightarrow P(\varepsilon) = C \times e^{-\delta \times \varepsilon/\Delta}$$

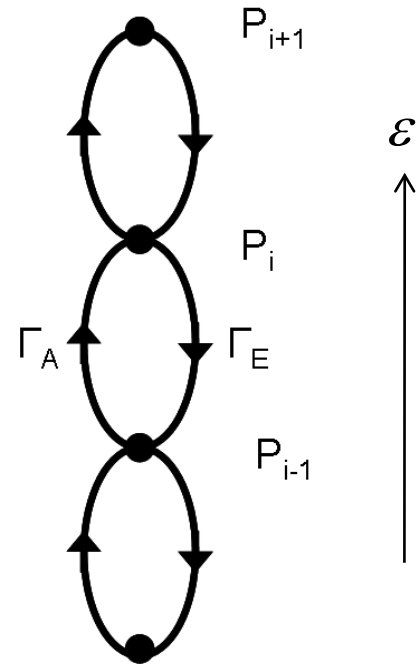


# Absorbing/Emitting phonons in Equilibrium

$$P(\varepsilon) = C \times e^{-\delta \times \varepsilon / \Delta}$$

Detailed balance …

$$\left.\begin{aligned} \frac{\Gamma_A}{\Gamma_E} &= e^{-\Delta/k_B T} \approx 1 - \frac{\Delta}{k_B T} \\ \frac{\Gamma_A}{\Gamma_E} &= \frac{\Gamma_0 (1-\delta/2)}{\Gamma_0 (1+\delta/2)} = 1-\delta \end{aligned}\right\} \quad \delta = \frac{\Delta}{k_B T}$$




$$P(\varepsilon_i) = C \times e^{-\varepsilon_i / k_B T}$$ and C by normalization $$\sum_i p(\varepsilon_i) = 1$$

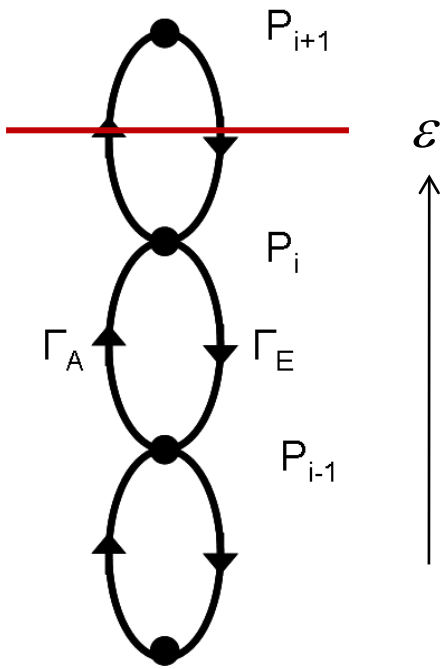
Approximate Bose-Einstein distribution

# Net flux in Equilibrium

$$F = (i+1)\Gamma_A P_i - i\Gamma_E P_{i+1}$$

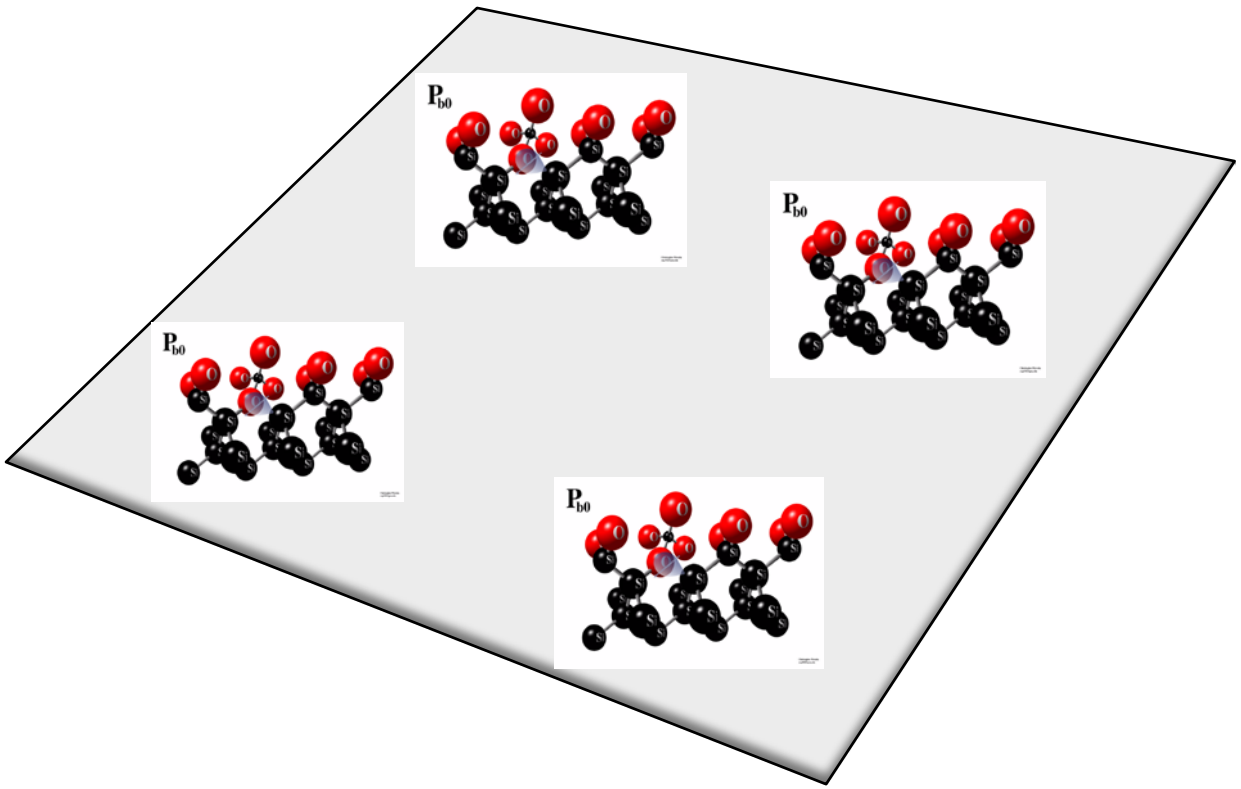
$$= (i+1)\Gamma_A P_i \left(1 - \frac{\Gamma_E}{\Gamma_A}\frac{P_{i+1}}{P_i}\right)$$

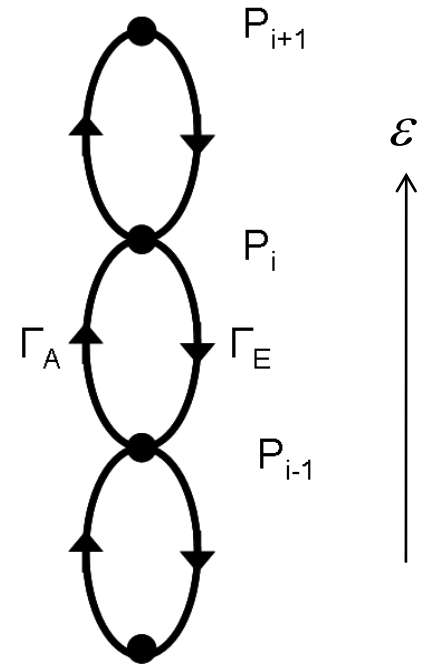
$$= (i+1)\times\Gamma_A P_i \left(1 - e^{\frac{\Delta}{k_B T}} \frac{e^{-\frac{\Delta\times(i+1)}{k_B T}}}{e^{-\frac{\Delta\times(i)}{k_B T}}}\right) = 0$$




… as expected.

# Meaning of the distribution …



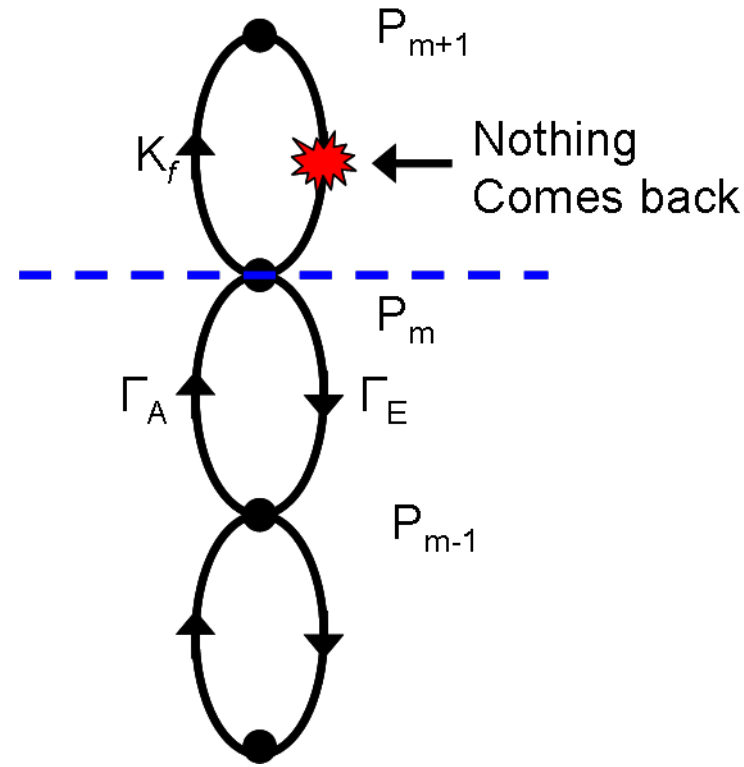
# Interpretation

Probability that a Si-H climbs the barrier

… that it finally absorbs a phonon to break the bond

$$F = (n_{\max} + 1) \times \Gamma_A \times e^{-\frac{E_F}{k_B T}}$$

$$\equiv k_{F0} \times e^{-\frac{E_{F0}}{k_B T}}$$



# Hot carrier induced dissociation

In thermal equilibrium …

$$\Gamma_A^{(0)} = \Gamma_E^{(0)} \times e^{-\frac{\hbar\omega_0}{k_B T}}$$

Rates with injected current …

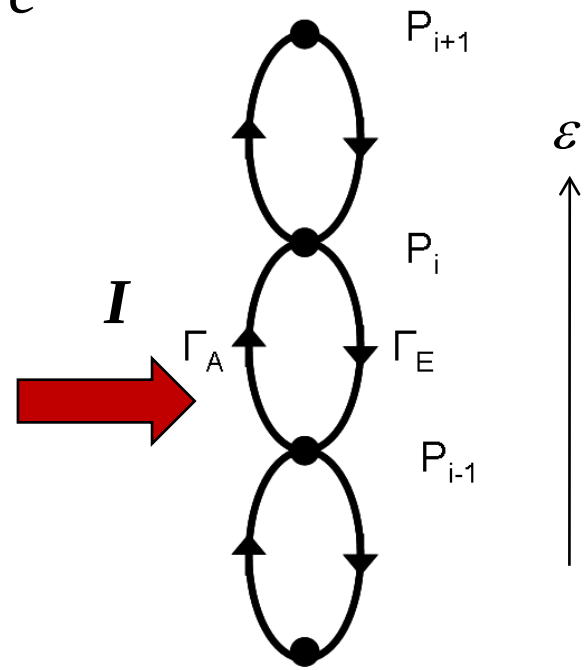
$$\Gamma_A = \Gamma_A^{(0)} + (I/q) f_{in} \qquad \Gamma_E = \Gamma_E^{(0)} + (I/q) f_{in}$$

Dissociation rates of Si-H bonds …

$$F = (n_{\max} + 1) \times \Gamma_A \left[ \Gamma_A / \Gamma_E \right]^{n_{\max}} \qquad n_{\max} \equiv \frac{E_F}{\Delta} = \frac{E_F}{\hbar\omega}$$

$$= (n_{\max} + 1) \times \Gamma_A \left[ \frac{\Gamma_A^{(0)} + (I/q) f_{in}}{\Gamma_E^{(0)} + (I/q) f_{in}} \right]^{n_{\max}}$$

$$\approx (n_{\max} + 1) \times \Gamma_A \left[ \frac{\Gamma_E^{(0)} e^{-\frac{\Delta}{k_B T}} + (I/q) f_{in}}{\Gamma_E^{(0)} + (I/q) f_{in}} \right]^{n_{\max}} \approx (n_{\max} + 1) \times \frac{\left[ (I/q) f_{in} \right]^{n_{\max}+1}}{\left( \Gamma_E^{(0)} \right)^n}$$




*Salam, PRB, 1994.*

# Hot carrier induced dissociation

In thermal equilibrium …

$$\Gamma_A^{(0)} = \Gamma_E^{(0)} \times e^{-\frac{\hbar\omega_0}{k_B T}}$$

Rates with injected current …

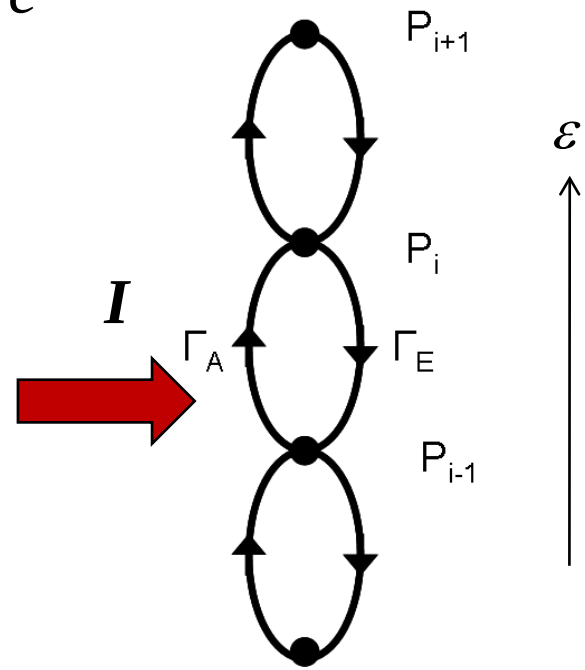
$$\Gamma_A = \Gamma_A^{(0)} + (I/q) f_{in} \qquad \Gamma_E = \Gamma_E^{(0)} + (I/q) f_{in}$$

Dissociation rates of Si-H bonds …

$$F = (n_{\max} + 1) \times \Gamma_A \left[ \Gamma_A / \Gamma_E \right]^{n_{\max}} \qquad n_{\max} \equiv \frac{E_F}{\Delta} = \frac{E_F}{\hbar\omega}$$

$$= (n_{\max} + 1) \times \Gamma_A \left[ \frac{\Gamma_A^{(0)} + (I/q) f_{in}}{\Gamma_E^{(0)} + (I/q) f_{in}} \right]^{n_{\max}}$$

$$\approx (n_{\max} + 1) \times \Gamma_A \left[ \frac{\Gamma_E^{(0)} e^{-\frac{\Delta}{k_B T}} + (I/q) f_{in}}{\Gamma_E^{(0)} + (I/q) f_{in}} \right]^{n_{\max}} \approx (n_{\max} + 1) \times \frac{\left[ (I/q) f_{in} \right]^{n_{\max}+1}}{\left( \Gamma_E^{(0)} \right)^n}$$




*Salam, PRB, 1994.*

# Appendices

1. Derivation of forward and reverse dissociation
2. Bose Einstein vs. Boltzmann distribution
3. Theory of Dispersive diffusion
4. Conclusion

# Appendix 2: Blocking factors

Phonons are Bosons, therefore in principle, we should include

$$\Gamma_A P_{i-1}(1+P_i)+\Gamma_E P_{i+1}(1+P_i)=\Gamma_A P_i\,(1+P_{i+1})+\Gamma_E P_i(1+P_{i-1})$$

$$\Gamma_A=\Gamma_0\left(1-\frac{\delta}{2}\right) \qquad \Gamma_E=\Gamma_0\left(1+\frac{\delta}{2}\right)$$

Corresponding differential equation …

$$\frac{d^2P}{d\varepsilon^2}+\frac{\delta}{\varepsilon_0}\left(\frac{1}{2}+P\right)\frac{dP}{d\varepsilon}=0 \quad with$$

$$\frac{dP}{d\varepsilon}=\frac{P_{i+1}-P_{i-1}}{2\varepsilon_0} \quad and \quad \frac{d^2P}{d\varepsilon^2}=\frac{P_{i+1}+P_{i-1}-2P_i}{2\varepsilon_0{}^2}$$

# Appendix 2: Blocking factors

$$\frac{d^2P}{d\varepsilon^2} + \frac{\delta}{\Delta}\left(\frac{1}{2} + P\right)\frac{dP}{d\varepsilon} = 0$$

$$P(\varepsilon) = \frac{1}{2}\frac{1}{e^{b\varepsilon} - 1}$$

Bose-Einstein distribution …

$$P(\varepsilon) = \frac{1}{2}\frac{1}{e^{\varepsilon/k_B T} - 1}$$

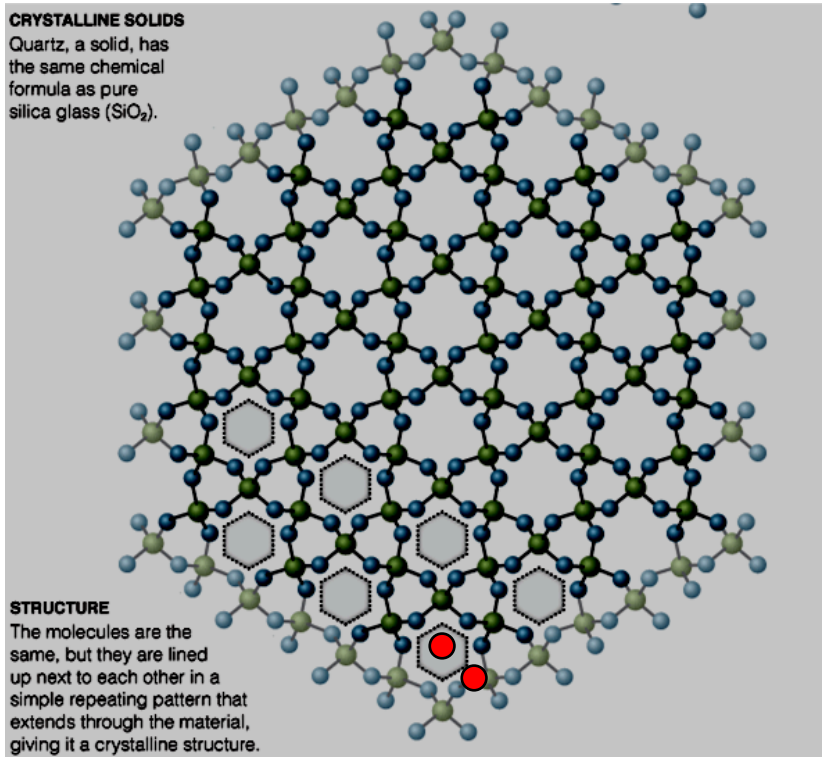
Maxwell-Boltzmann dist …

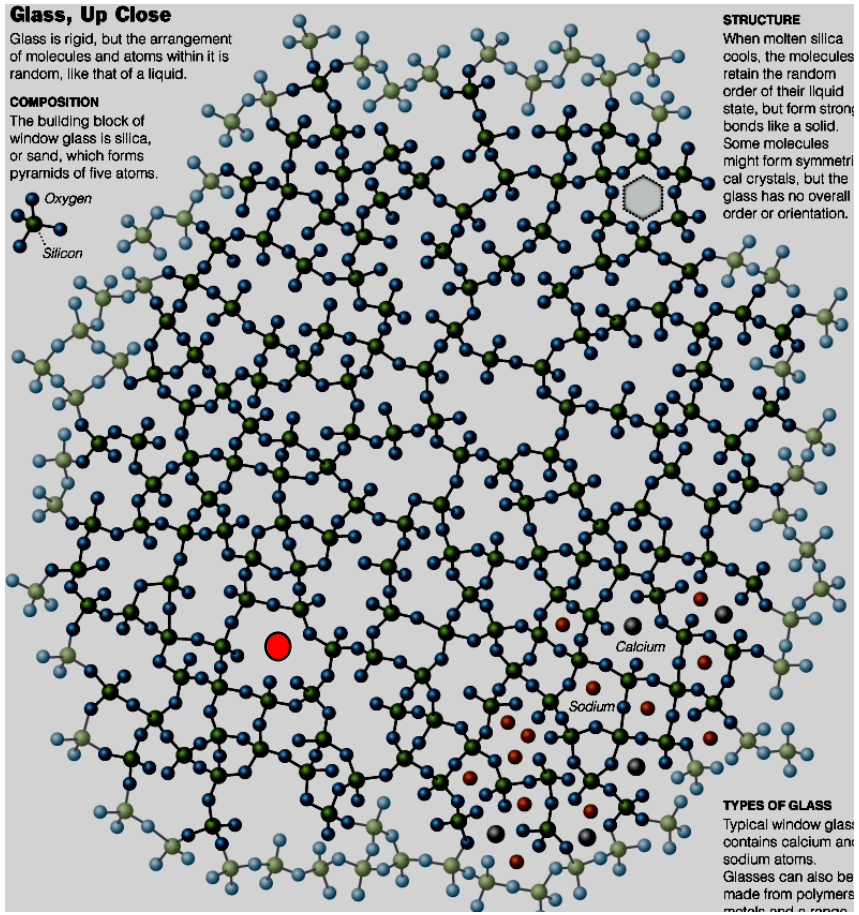
$$P(\varepsilon \to \infty) \sim Ae^{-\frac{\varepsilon}{k_B T}}$$

# Appendices

1. Derivation of forward and reverse dissociation
2. Bose Einstein vs. Boltzmann distribution
3. Theory of Dispersive diffusion
4. Conclusion

# Appendix 3: Crystalline vs. Amorphous Oxides



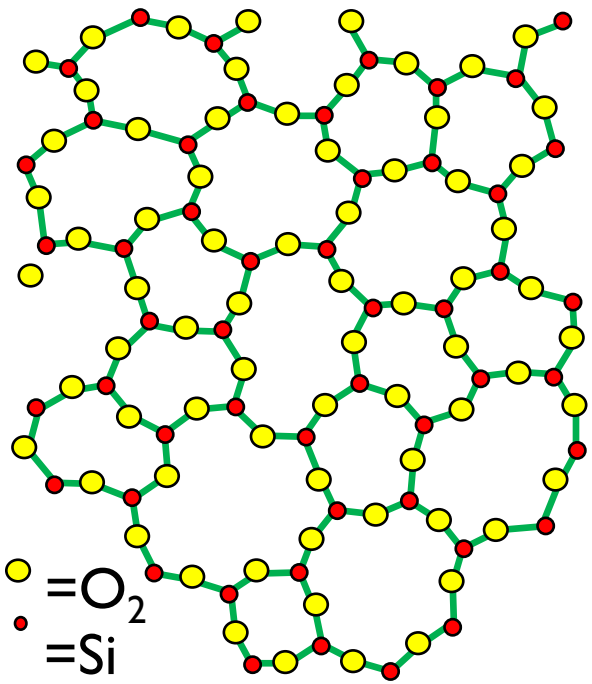



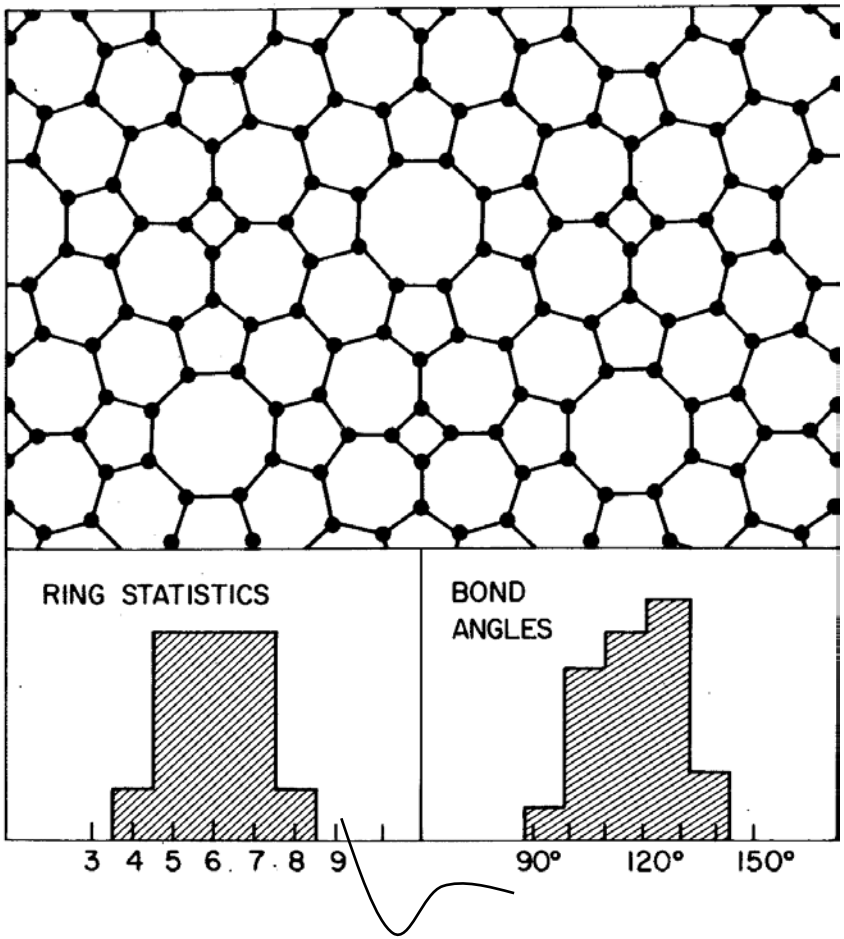

**'Glass up Close',**

*NY Times, July 29, 2008.*

# Ring size distribution

**Amorphous**

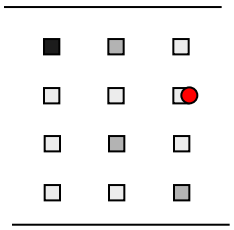



Exponentially few deep levels?

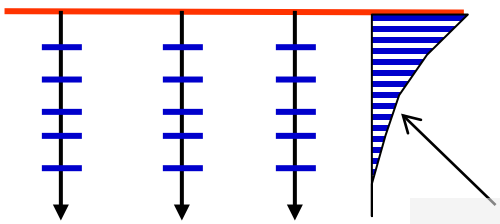
# Dispersive diffusion in amorphous material

Real-Space



Energy-Space

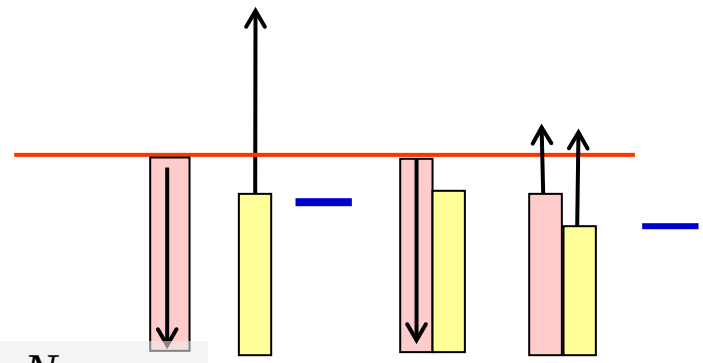
$$\frac{N_H^f}{N_B} = \frac{N_H^{b,i}}{N_{T,i}} \mathrm{e}^{-E_{T,i}/k_B T}$$



$$g(E) \equiv \frac{N_T}{E_0} e^{-E/E_0}$$

Moment-Space

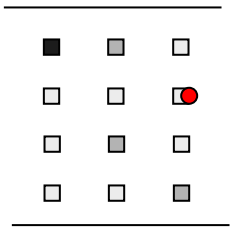
$$\tau_e^{-1}(E_T) = \nu e^{-E_T(t)/k_B T} = t^{-1}$$



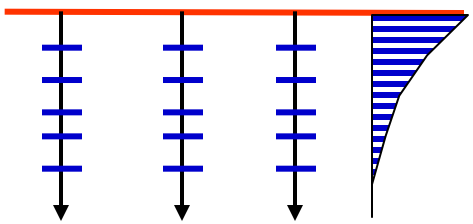
$$\frac{N_H^f}{N_H^b} = \frac{N_B \, \mathrm{e}^{-E_T(t)/kT}}{E_0 \frac{N_T}{E_0} e^{\frac{-E_T(t)}{E_0}}} = \frac{N_B e^{\frac{-k_B T \ln(\nu t)}{k_B T}}}{N_T e^{\frac{-k_B T \ln(\nu t)}{E_0}}} = \frac{N_B}{N_T} \left( \frac{1}{\nu t} \right)^{1 - \frac{k_B T}{E_0}}$$

# Dispersive diffusion in amorphous material

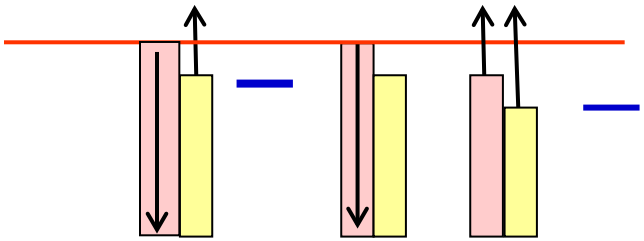
Real-Space



Energy-Space



Moment-Space



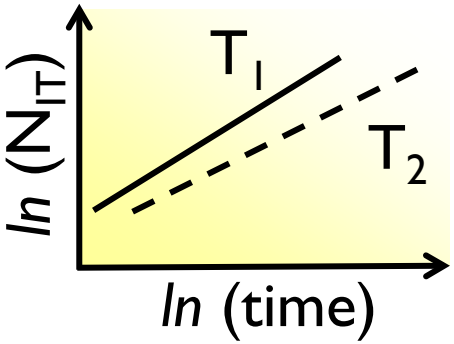
$$\frac{dN_{IT}}{dt} = D_0^* \frac{d^2 N_H^f}{dx^2}$$

$$N_H^f = N_B \frac{N_H^b}{N_T} \left(\frac{1}{vt}\right)^{1-\frac{k_B T}{E_0}}$$

$$\Rightarrow \frac{dN_{IT}}{dt} = D_H \frac{d^2 N_H}{dx^2} \square D_H \frac{d^2 N_H^b}{dx^2}$$

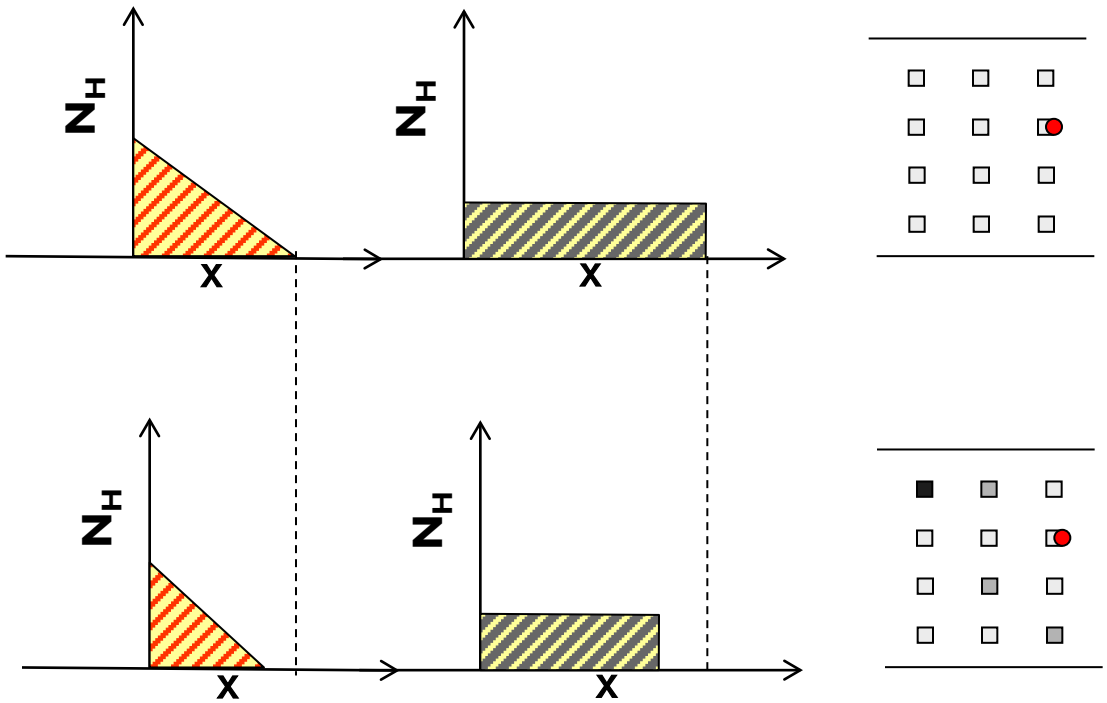
$$D_H \equiv D_0 \left(\frac{1}{vt}\right)^{\left(1-\frac{k_B T}{E_0}\right)}$$

$$D_0 = D_0^* \frac{N_B}{N_T}$$




*Orenstein, PRL, 46, 1421, 1981*

# Dispersive diffusion: effect on time exponent




$$N_{IT}(t) \propto \sqrt{\frac{k_F N_0}{2k_R}} (D_{H_*} t)^n$$

$$D_H = D_0 (vt)^{-p}$$

*Shkrob, PRB, 1996; 54:15073*

$$N_{IT}(t) \propto \sqrt{\frac{k_F N_0}{2k_R}} \left(\frac{D_0}{v^p}\right)^n t^{n(1-p)}$$

| | $n_{ideal}$ | $n_{dis}$ |
|---|---|---|
| H | 0.25 | 0.20-0.25 |
| H2 | 0.16 | 0.128-0.144 |
| H2+ | 0.33 | 0.264-0.297 |

# Dispersive diffusion with finite traps

Ratio of free vs. trapped H changes upto a point ….

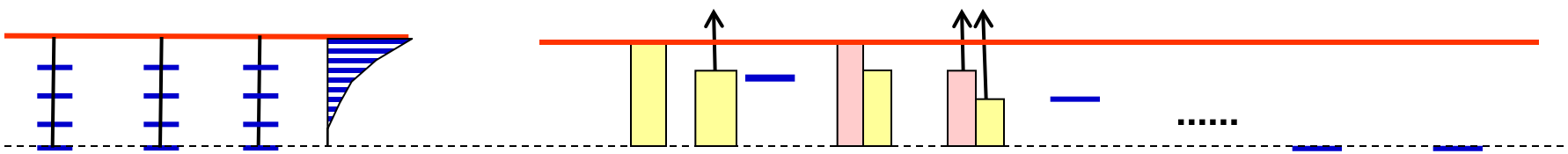
Energy-Space

$$\frac{N_H^f}{N_B} = \frac{N_H^{b,i}}{N_{T,i}} e^{-E_{T,i}/kT}$$

Moment-Space

$$\frac{N_H^f}{N_B} = \frac{N_H^b \, e^{-E_T(t)/k_B T}}{E_0 g(E_T)}$$

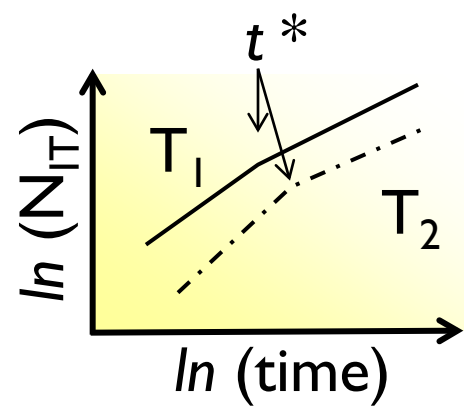
$$\frac{N_H^f}{N_B} \sim \frac{N_H^b \, e^{-E_T^*/kT}}{E_0 g(E_T^*)}$$




$$\frac{dN_{IT}}{dt} = D_0^* \frac{d^2 N_H^f}{dx^2} \Rightarrow \frac{dN_{IT}}{dt} = D_H \frac{d^2 N_H}{dx^2}$$

$$D_H = D_0 (1/\nu t)^{(1-k_B T/E_0)} \qquad 0 < t < t^*$$

$$= D_0 e^{-Ea/k_B T} \qquad t^* < t$$



# Dispersive in time exponent: Multi level traps

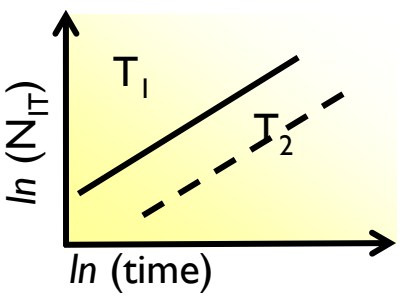
$$N_{IT} \square \left(D_H t\right)^n$$

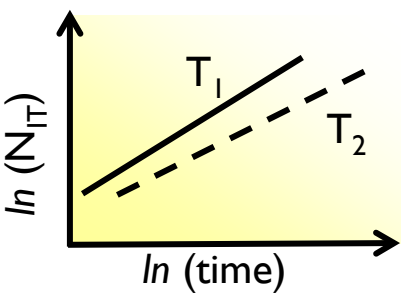
Activated diffusion

$$N_{IT} \propto \left[ D_0 e^{-\frac{E_a}{k_B T}} t \right]^n = \left(D_0\right)^n e^{-\frac{nE_a}{k_B T}} \times t^n$$

Dispersive diffusion

$$N_{IT} \propto \left[ D^* \left(\frac{N_c}{E_0}\right) \left(\frac{1}{\nu t}\right)^{1-\frac{kT}{E_0}} t \right]^n \sim t^{\frac{nkT}{E_0}}.$$



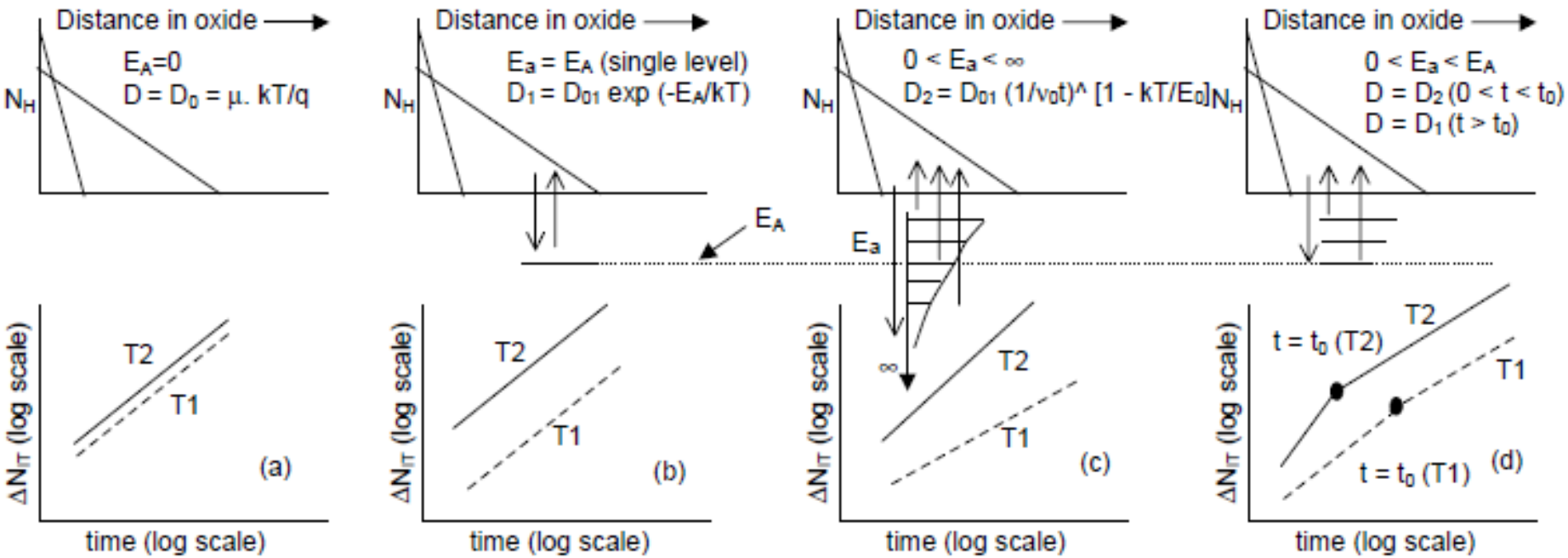



# Aside: Dispersive/subdiffusion and fractional calculus

*Fractional Kinetics, I. Sokolov, J. Klafter, and A. Blumen*

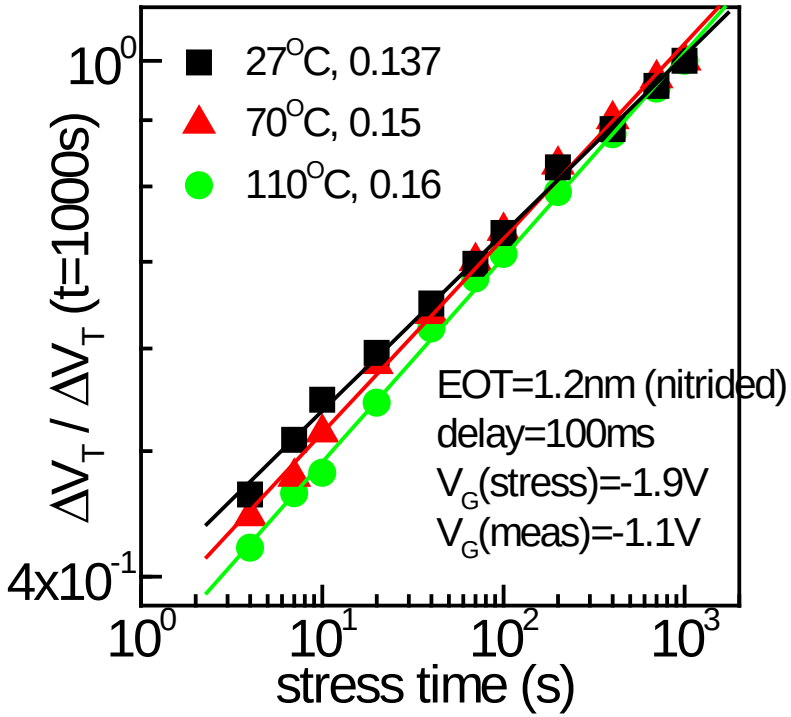
*Physics Today, Nov. 2002, page. 48.*

# Summary of temperature activation




*Ref. D.Varghese, IEDM 2005*

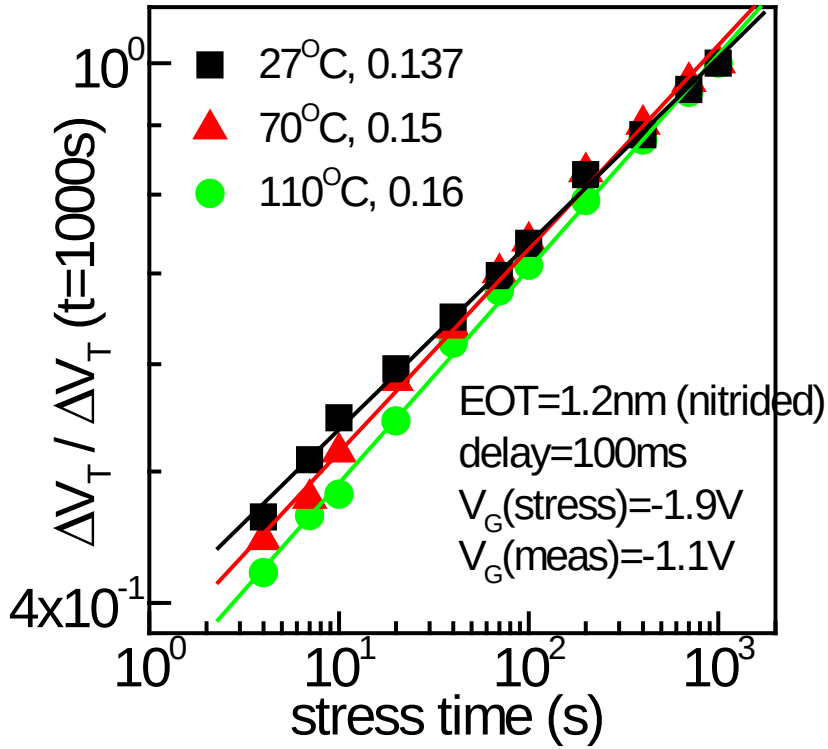
# Temp. dependence: activation vs. dispersion



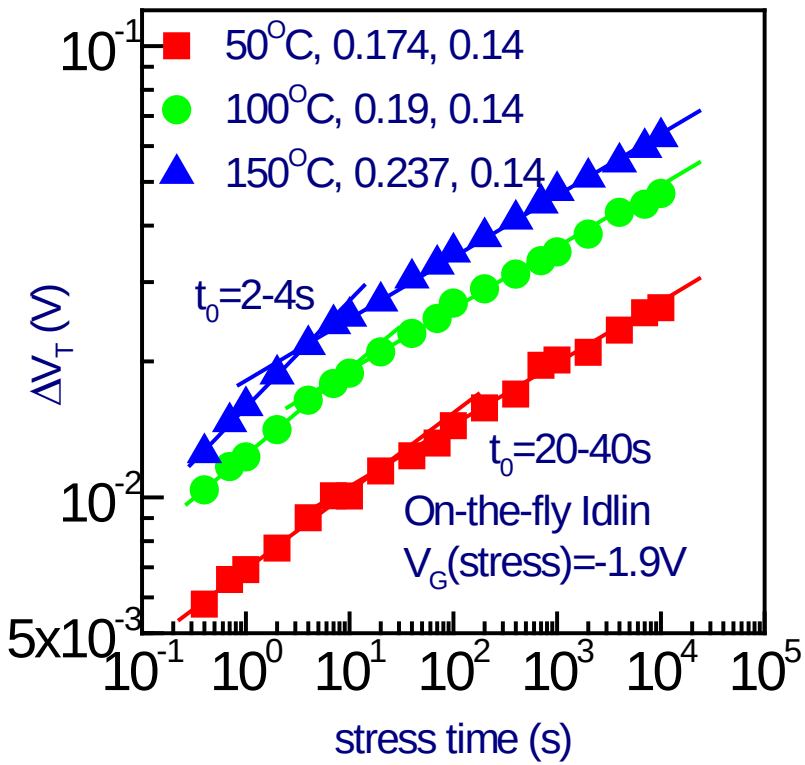

Can we even define an activation energy …. ?

# Temperature dependent dispersion

with delay ….

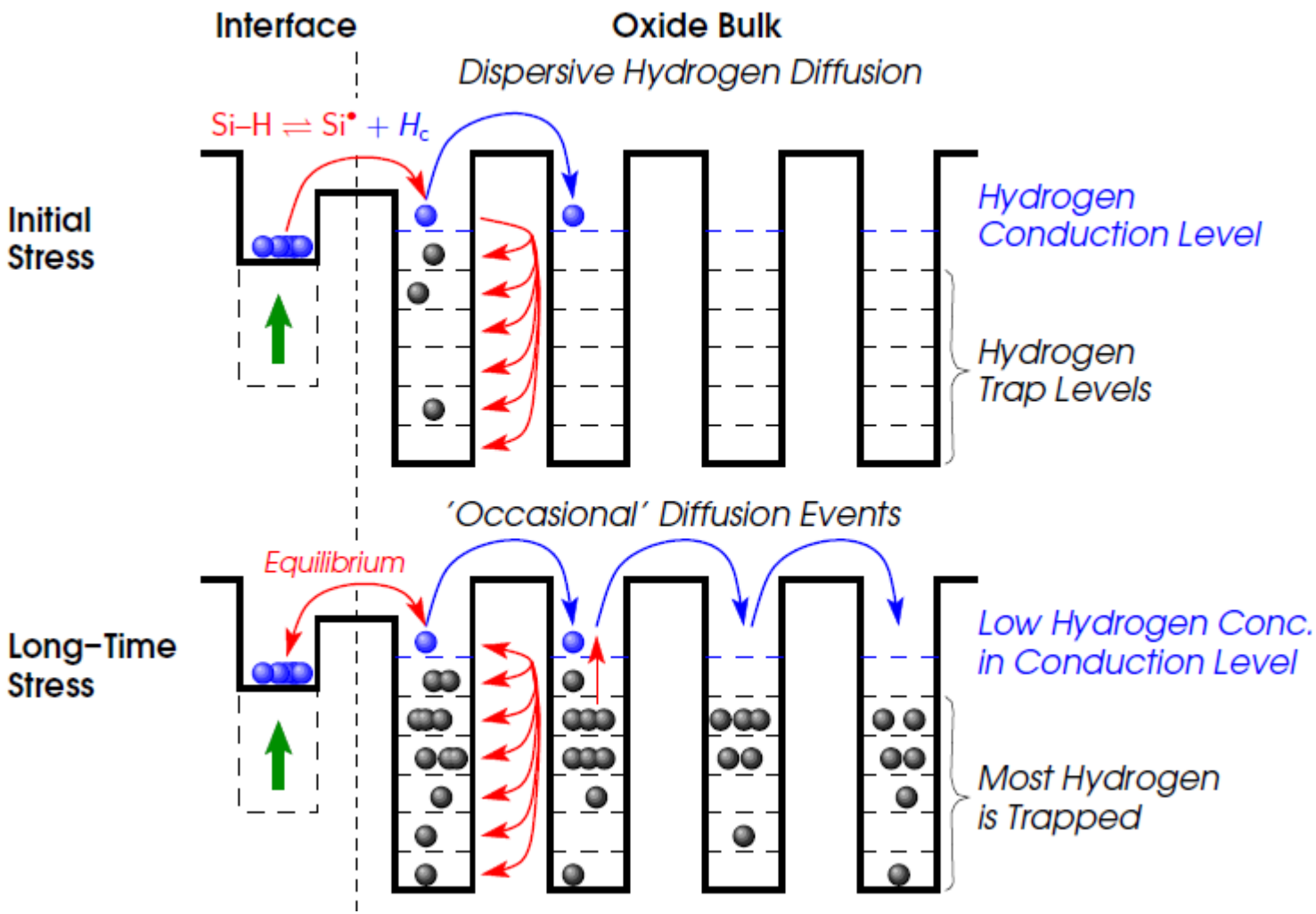



without delay ….



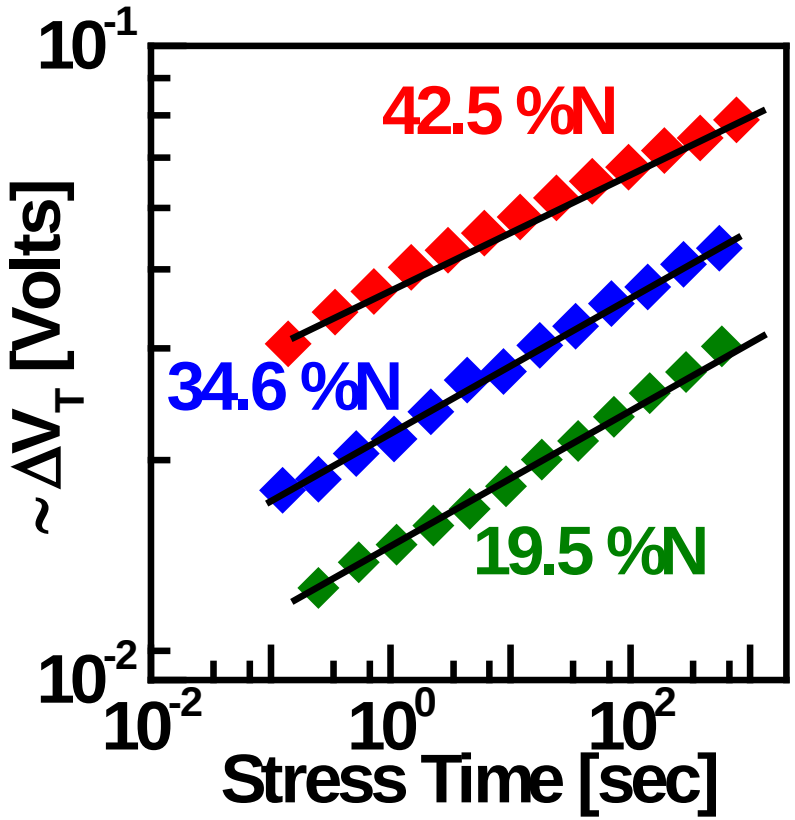

- Transition time reduces with increase in T
- Transition from dispersive to activated diffusion ($E_0$=80meV, $n_0=10^{12}s^{-1}$)

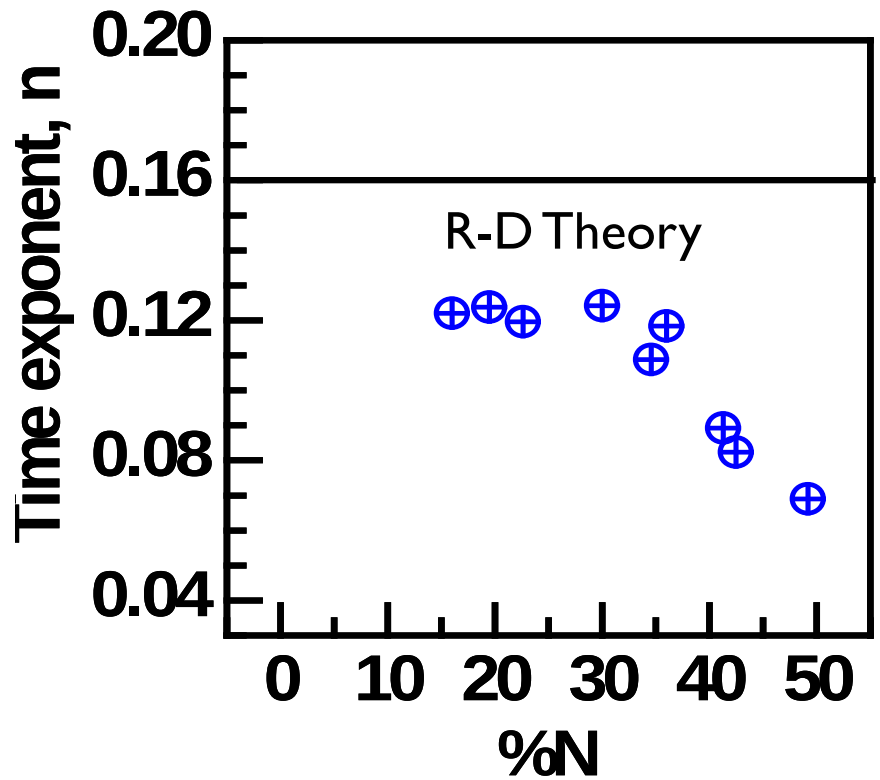
# Temperature dissociation of Si-H bonds




*Taken from T. Grasser, IRPS Tutorial, 2007.*

# NBTI signatures: stress time

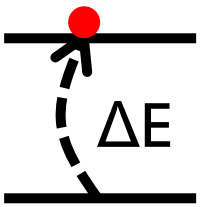



- Universal existence of power-law at long $t_{STS}$
- Time exponent reduces with %N

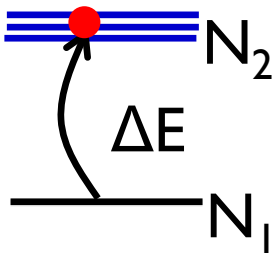
# Aside: Where is the Entropy?
# Energy vs. Free energy

Transition rates, $R \propto e^{-\Delta E / K_B T}$




Transition rates,

$$R \propto N \times e^{-\Delta E / K_B T}$$




$$= e^{-\frac{\Delta E}{K_B T} + \frac{T \times K_B \ln(N)}{K_B T}} \equiv e^{-\frac{\Delta E}{K_B T} + \frac{\Delta S T}{K_B T}}$$

$$= e^{-\frac{\Delta E - T \Delta S}{K_B T}} \equiv e^{-\frac{\Delta F}{K_B T}}$$

$$k_F = \underbrace{k_{F0}}_{} \times e^{-\frac{E_{FO}}{k_B T}}$$

This has the state density

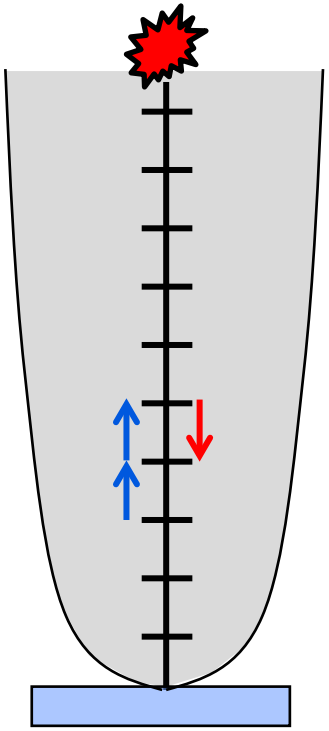
Entropy,

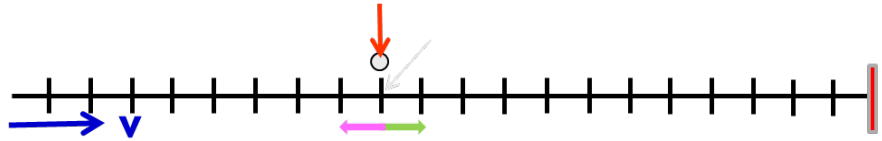
$$S \equiv k_B \ln(N)$$

Free energy,

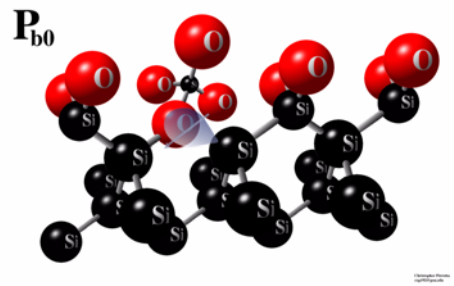
$$F \equiv E - ST$$

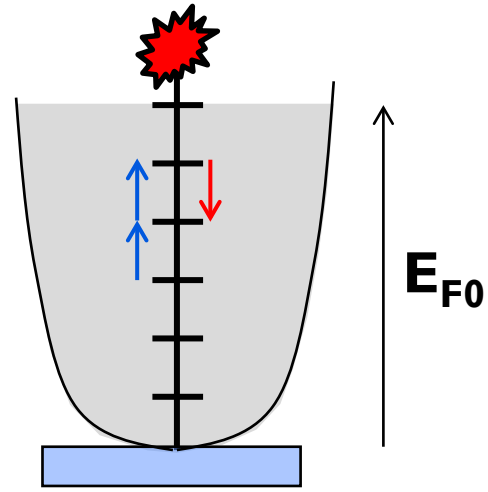
# BFRW Analogy for dissociation rate






accelerate $q = 0.5(1-\Delta(\upsilon))$ $p = 0.5(1+\Delta(\upsilon))$




Before hole capture

After hole capture

$$F = \Gamma_0 \left(n_{\max} + 1\right) \times \Gamma_E \left[\frac{\Gamma_A}{\Gamma_E}\right]^{n_{\max}+1} \propto 1 \times \left[\frac{e^{-\hbar\omega/kT}}{1}\right]^{n_{\max}+1} \sim e^{-\frac{E_{F0}}{kT}}$$

Alam ECE 695

# Conclusion

- We have discussed the origin of temperature dependent activation of the dissociation rates and the diffusion coefficients.

- Diffusion in amorphous material may be dispersive – the diffusion coefficient changes depending on the filling-state of the defect. In thin films, dispersive diffusion may be relatively short.

- If films have too many pre-existing defects, the activation energy and the power-exponents may show non-ideal values. One should experimental data carefully.

- Fractional calculus has been extensively used for theory of anomalous diffusion …. Check it out.