

ECE695: Reliability Physics of Nano-Transistors

Lecture 16: Temperature dependence of HCI

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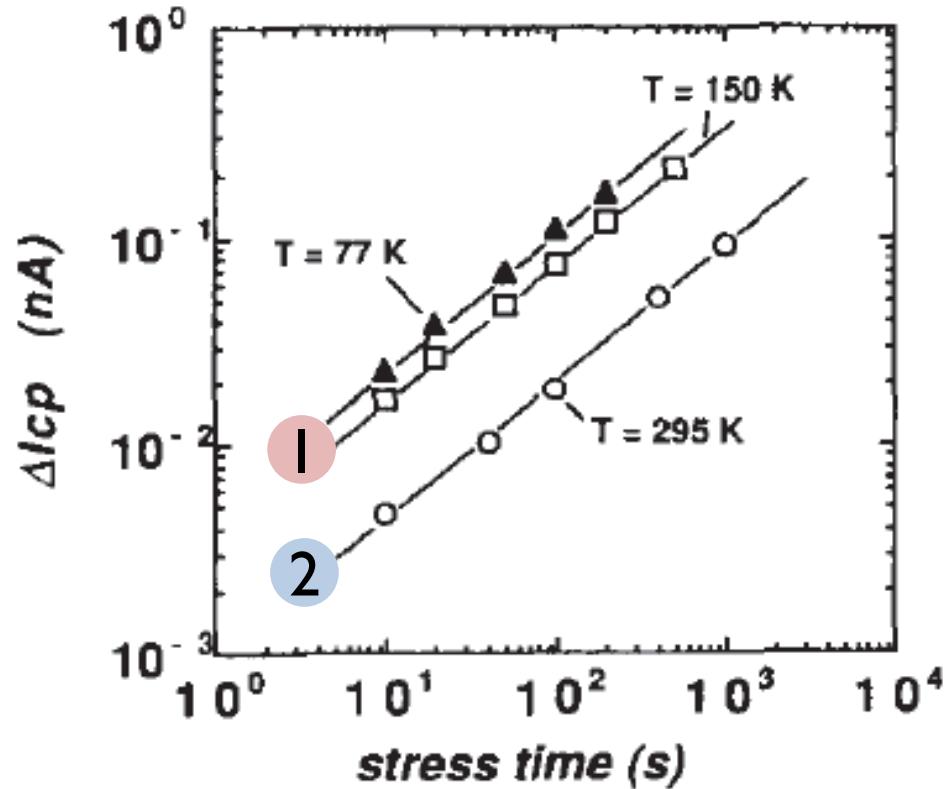
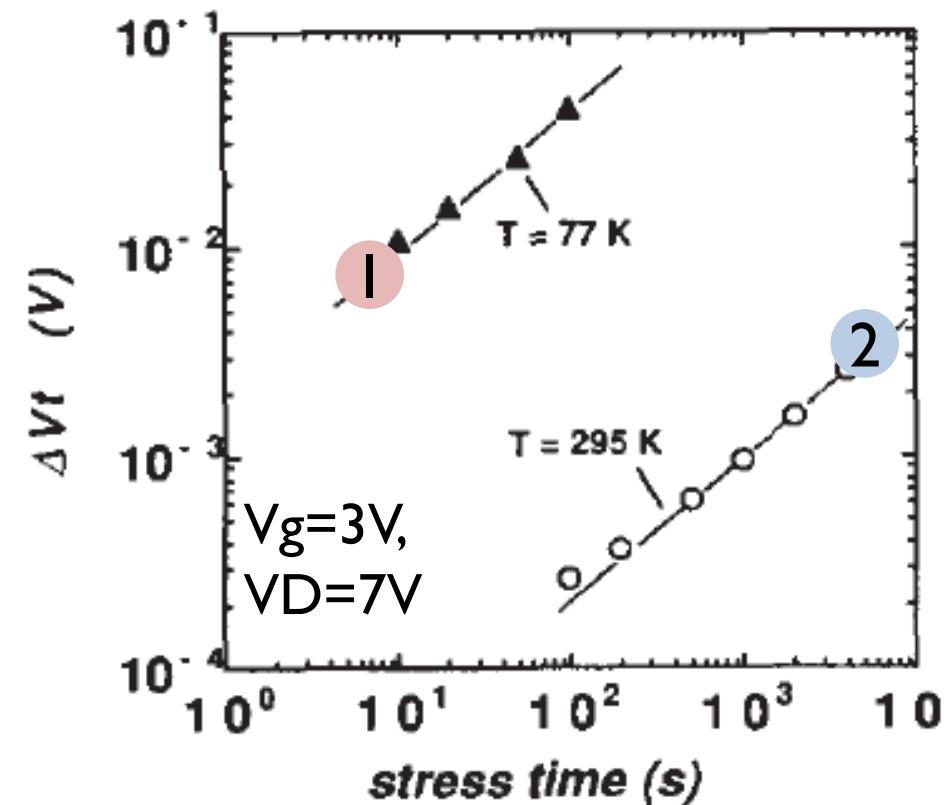
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Outline

- I. Empirical observations regarding HCl
2. Theory of bond dissociation: MVE vs. RRK
3. Hot carrier dissociation of SiH bonds
4. Hot carrier dissociation of SiO bonds
5. Conclusions

Empirical observations (1)

P. Heremans, TED, 37(4), p. 980, 1990.



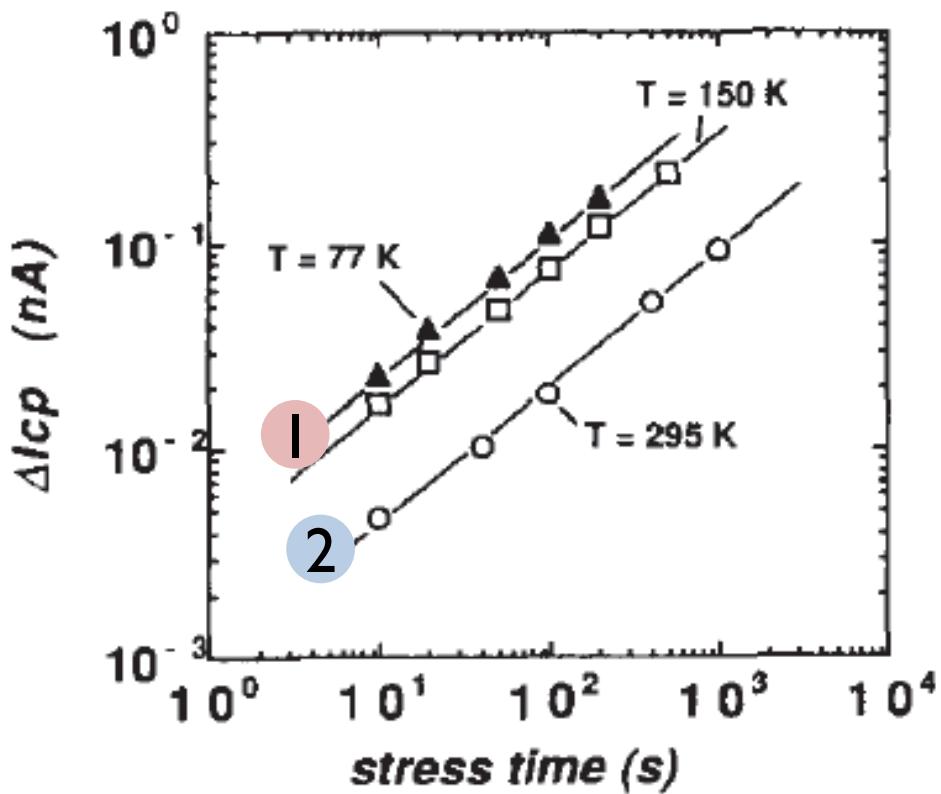
Less VT degradation at higher temperature

$I_{cp} \sim N_{it}$ and Not confirms trap generation

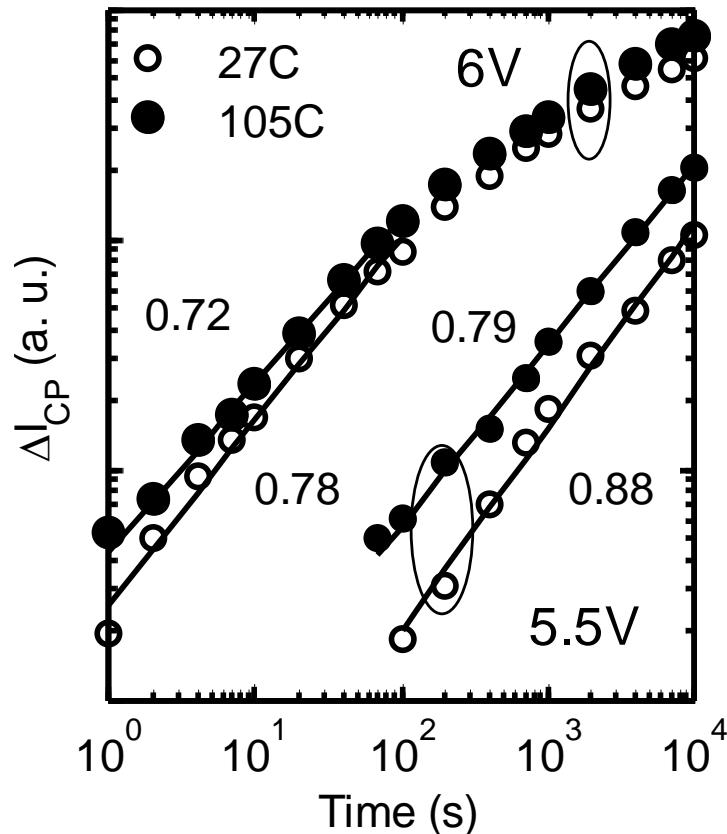
After dE correction, N_{it} could be larger at higher temperature

Empirical Observation (2)

P. Heremans, TED, 37(4), p. 980, 1990.



Robust exponent,
SiH dissociation ?

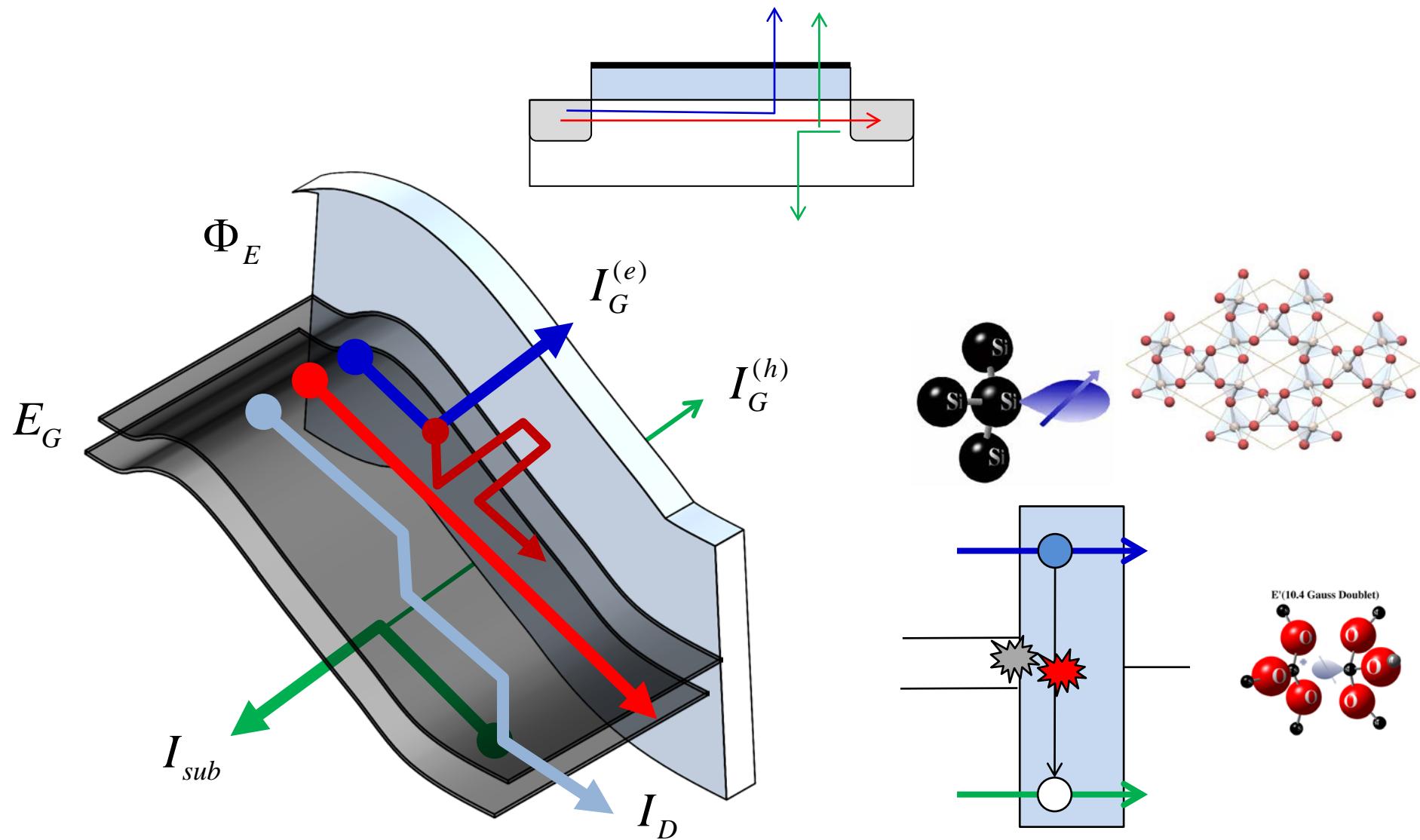


Variable exponent
SiO dissociation ?

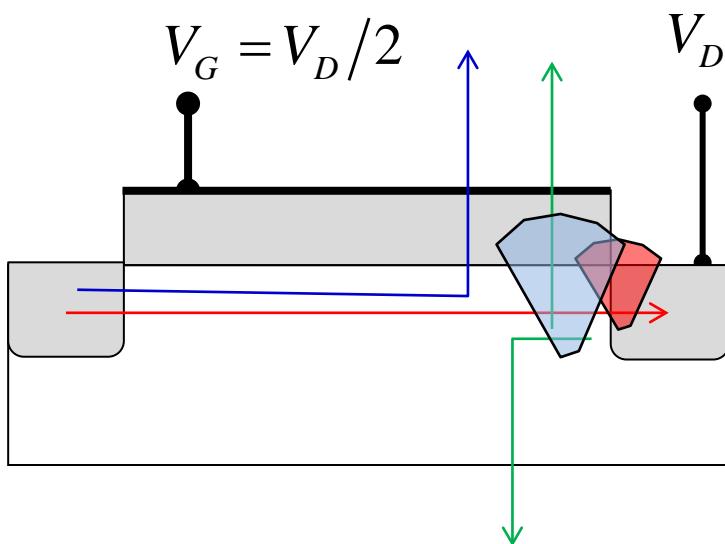
Outline

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A model for HCl degradation



HCl: Temperature dependence



Carriers are no longer cold

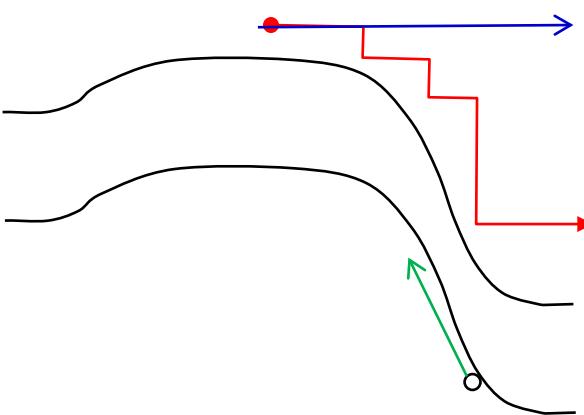
(1) Electrons heated by field

SiH dissociation...

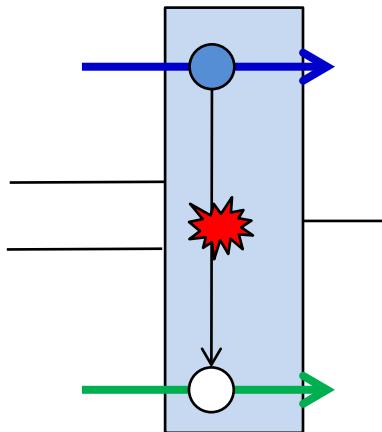
(2) Heating of electrons
Hot electrons break SiH bonds

SiO dissociation...

(3) Hot electron produces
Hot holes through II
Hot are trapped in oxide
Electron-hole recombination
breaks bonds

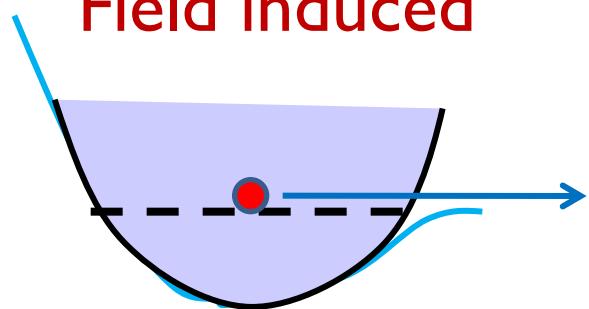


Dissociation by energy flow: What happened to activation of bond dissociation



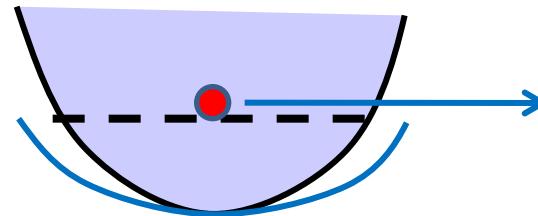
Kimerling, SSE, 21, 1391, 1978.

Field induced



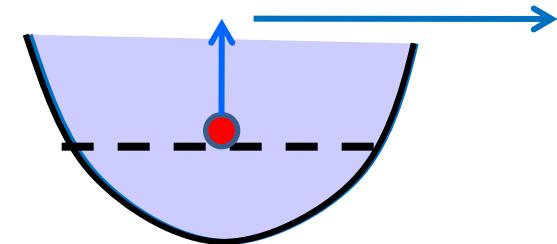
NBTI, TDDB

Charge State



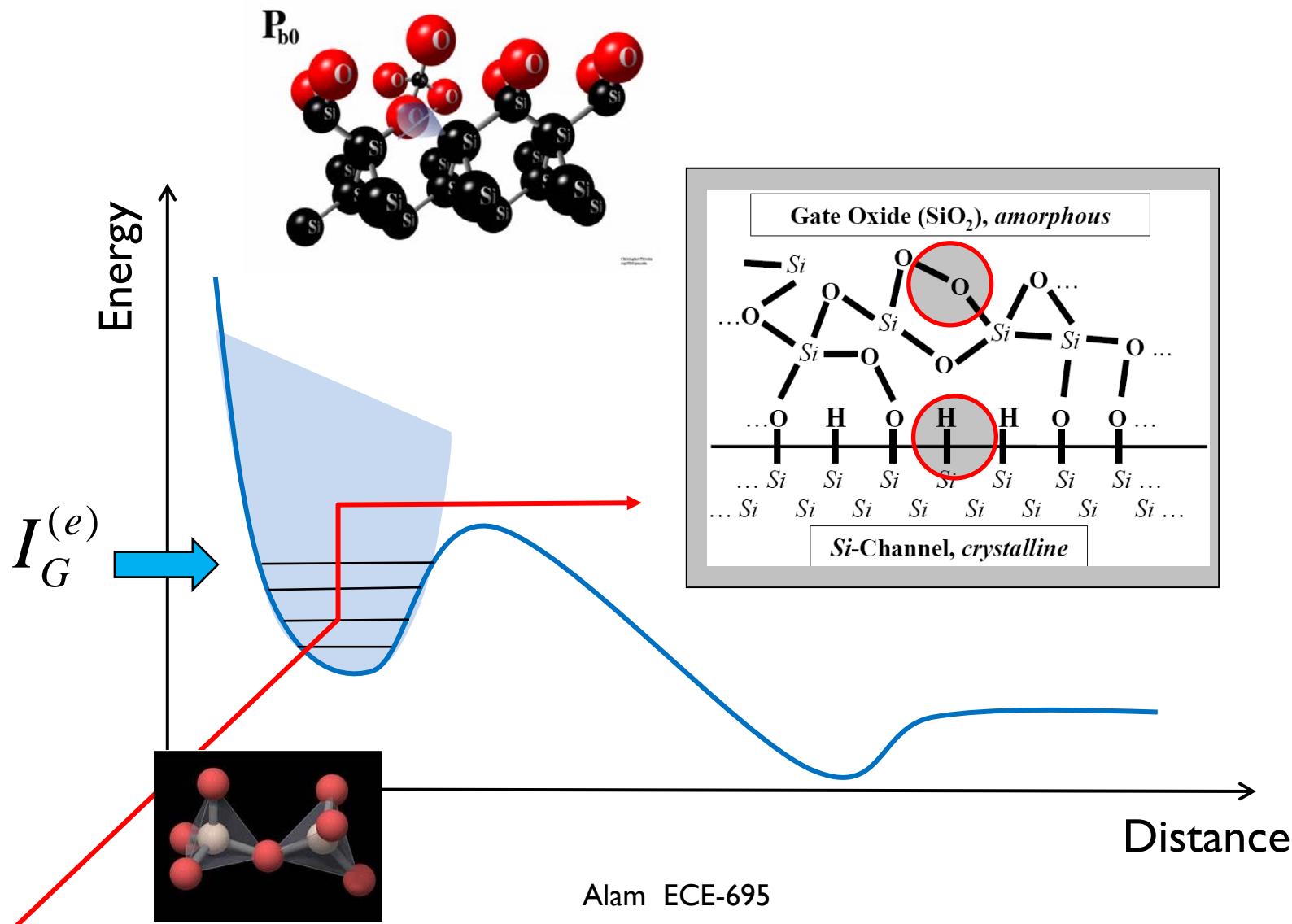
NBTI primarily

Energy driven or
e-h recombination



HCI, TDDB, etc.

Dissociation of Si-H or Si-O bonds



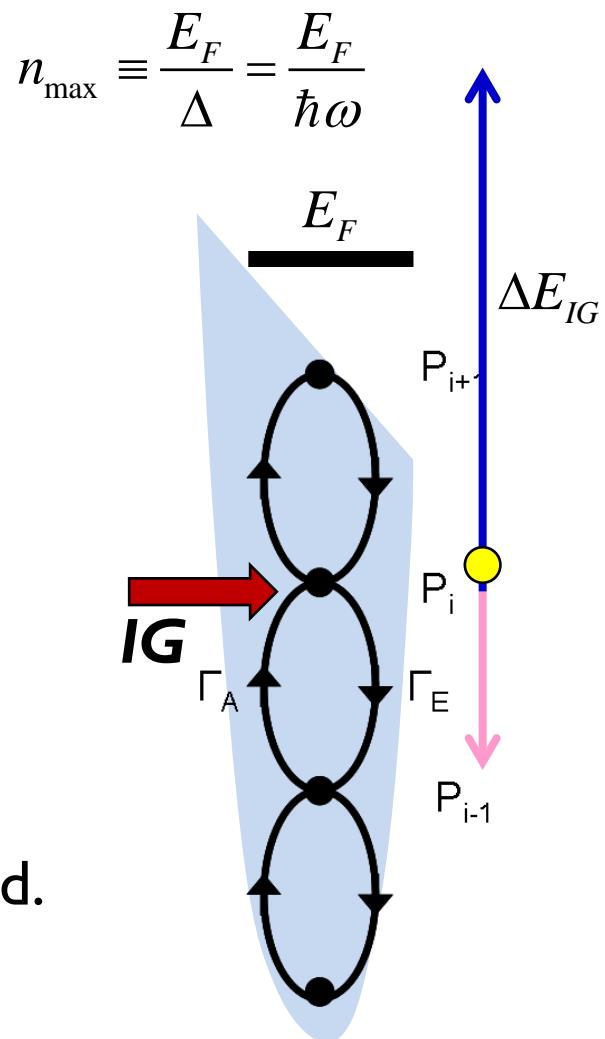
Bond dissociation: RRK Theory

Recall from **lecture 11** that

$$k_F^{(\text{NBTD})} \approx (n_{\max} + 1) \times \Gamma_A \left(\frac{\Gamma_A^{(0)}}{\Gamma_E^{(0)}} \right)^{n_{\max}} \sim k_{F_0} e^{-\frac{E_F}{kT_L}}$$

$$k_F^{(\text{HCl})} \approx \left(f_{in} \frac{I_G(T_L) \downarrow}{q} \right) \times \left(\frac{e^{\frac{(E_F - \Delta E_{IG})}{kT_L}} \uparrow}{\Gamma_E(T_L) \uparrow} \right)$$

- Activation energy is considerably suppressed.
- Overall sign depends on current coupling



Weeks, Tully, Kimerling, PRB, 1975.

Bond dissociation at low voltages: Coherent Multi-Vibrational Excitation

Recall from **lecture II** that in thermal equilibrium ...

Rates with injected current ...

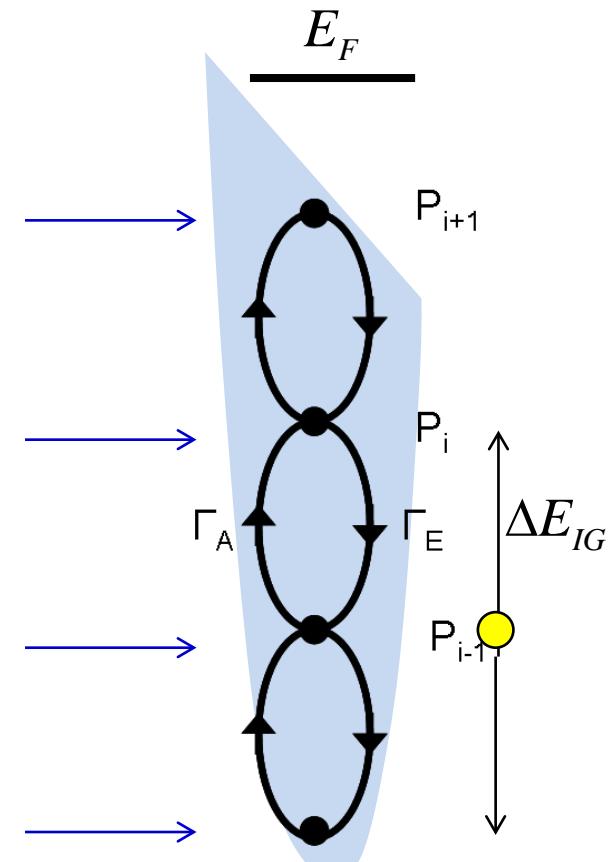
$$\Gamma_A = \Gamma_A^{(0)} + (I_G/q)f_{in} \quad \Gamma_E = \Gamma_E^{(0)} + (I_G/q)f_{in}$$

Dissociation rates of Si-H bonds ...

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

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

$$F_{HCl} (\propto k_F) \approx (n_{\max} + 1) \times \frac{\left[(I_G^{(e)}/q)f_{in} \right]^{n_{\max}}}{\left(\Gamma_E^{(0)} \right)^{n_{\max}}}$$



T.-C. Chen, Science, 1995.

Outline

- I. Empirical observations regarding HCl
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3. Hot carrier dissociation of SiH bonds
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5. Conclusions

HCI T-Dependence: Si-H Dissociation

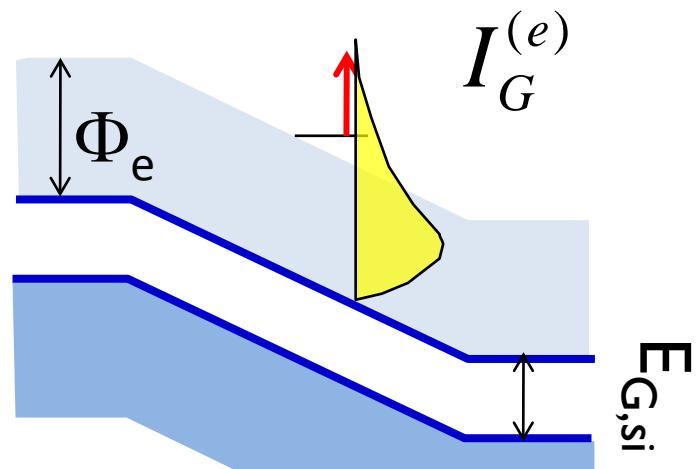
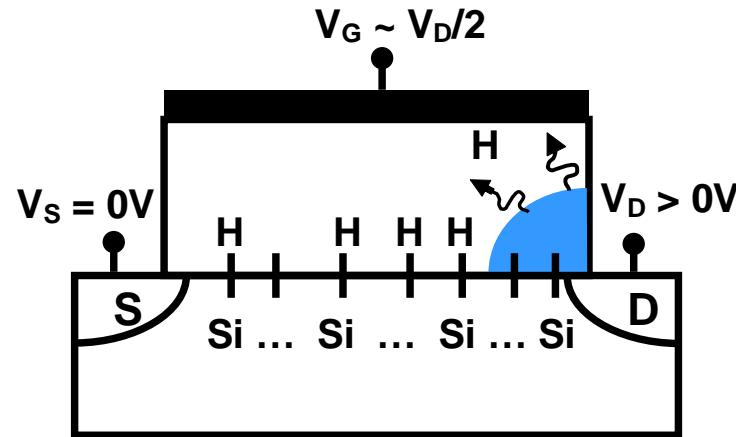
$$N_{IT} = \left(\frac{\pi}{3} \frac{k_F N_O}{k_R} \right)^{1/2} (D_H t)^{1/2} \dots \text{H model}$$

$$= \left(\frac{\pi}{6} \frac{k_F N_O}{k_R} \right)^{2/3} (D_{H_2} t)^{1/3} \dots \text{H}_2 \text{ model}$$

$$N_{IT} (.., T) \propto \left(\frac{k_F(T)}{k_R(T)} \right)^p [D_X(T)]^q$$

$$D_X(T) = D_0 e^{-E_D/kT} \quad k_R(T) = k_{R,0} e^{-E_R/kT}$$

$$\mathbf{k}_F = (I_G^{(e)}) \otimes g(E_F)$$



Recall: Field dependence of HCl

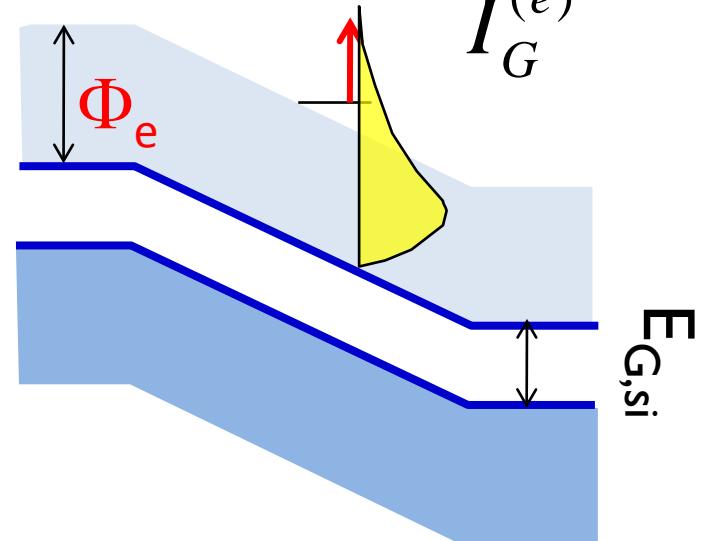
$$I_G^{(e)} = \int_0^l q n_0 \left(\frac{k_B T_e(x)}{2\pi m^*} \right)^{1/2} e^{\frac{-\Phi_e}{k_B T_e(x)}} dx.$$

$$\approx \frac{I_D}{v_{sat}} \left[l \sqrt{\frac{q \mathcal{E}_m \lambda_e}{m^*} \frac{U_0 q}{\Phi_e} \frac{\lambda_e}{l}} \right] e^{\frac{-\Phi_e}{q \mathcal{E}_m \lambda_e}}$$

$$\propto \frac{I_D}{v_{sat}} e^{-(\Phi_e l / q \lambda_e) / (V_D - V_{dsat})}$$

with $\lambda_e(T_L) = \left[\frac{2n_{ph}(T_{ref}) + 1}{2n_{ph}(T_L) + 1} \right] \lambda_e(T_{ref})$ $n_{ph}(T) \equiv [\exp(\hbar\omega/k_B T_L) - 1]^{-1}$

T-dependence of ID (through μ and V_T) and v_{sat} (through m) are weak..
 MFP decreases with lattice temperature, making injection difficult.



Dissociation of SiH bonds

$$k_{F,MVE}^{(\text{HCI})} \approx \left[(I_G^{(e)} / q) f_{in} \right]^{n_{\max}} / \left(\Gamma_E^{(0)} \right)^{n_{\max}}$$

$$\left(\Gamma_E^{(0)} \right)^{-n_{\max}} = Be^{-\frac{(DT) \times \frac{E_F}{\hbar\omega_0}}{}}$$

$$k_{F,RRK}^{(\text{HCI})} \approx \left(f_{in} \frac{I_G(T_L) \downarrow}{q} \right) \times \left(\frac{e^{\frac{(E_F - \Delta E_{I_G})}{kT_L}}}{\Gamma_E(T_L) \uparrow} \right)$$

$$\left(\Gamma_E^{(0)} \right) = Be^{-(DT)} \quad n_{\max} \equiv \frac{E_F}{\Delta} = \frac{E}{\hbar\omega}$$

Dissociation rates decreases rapidly with increase in temperature

Foley, PRL, 80(6), 1336 1998

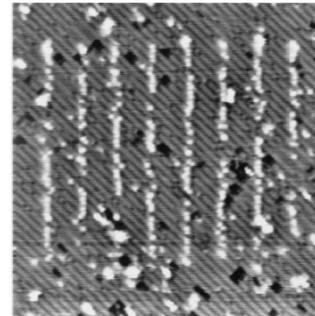
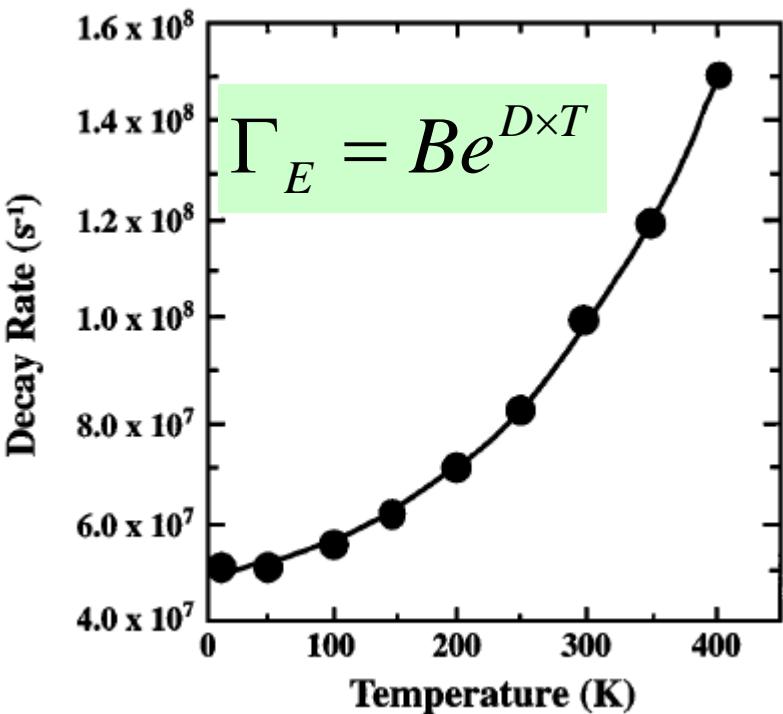


FIG. 1. A 400 Å × 400 Å image of a Si(100)-(2×1)H surface imaged at 11 K after threshold STM patterning of a series of parallel lines.

SiH T-Dependence: MVE Theory

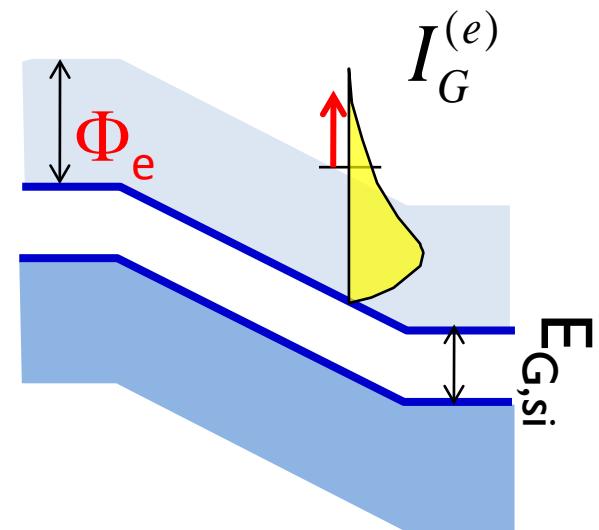
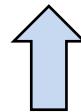
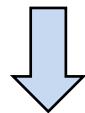
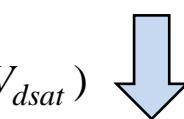
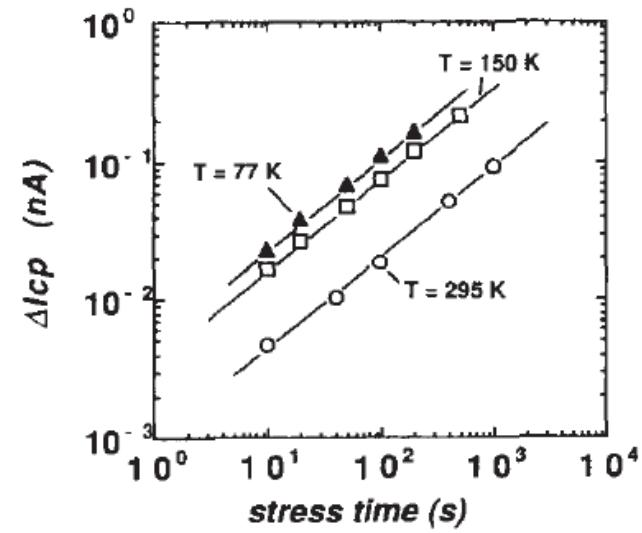
$$N_{IT} \propto \left(\frac{k_F N_O}{k_R} \right)^m (D_H t)^n$$

$$\propto (I_G F_{HCI})^m (D_H)^n$$

$$I_G \propto \frac{I_D}{V_{sat}} e^{-(\Phi_e l/q\lambda_e(\textcolor{red}{T}_L))/(V_D - V_{dsat})}$$

$$F_{HCI} \propto \left(\Gamma_E^{(0)} \right)^{-n} = B e^{-\frac{DE_F}{\hbar\omega_0} \textcolor{red}{T}_L}$$

$$D_H \equiv D_0 e^{-E_A/k_B \textcolor{red}{T}_L}$$

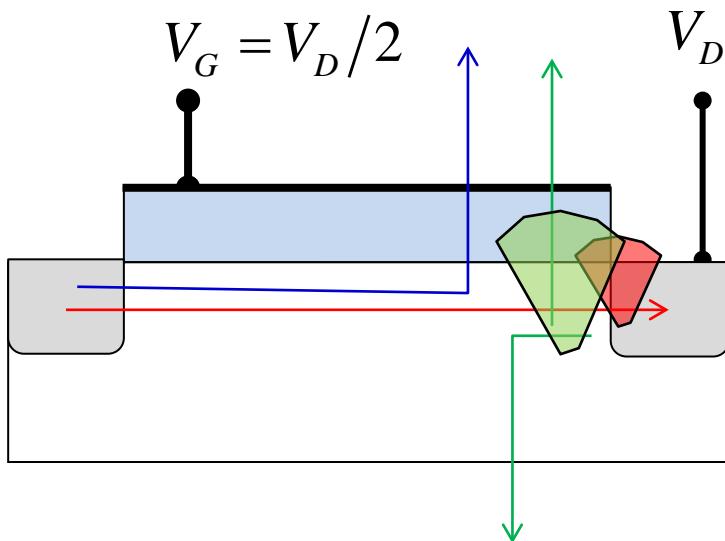


Taken together, the SiH bond dissociation is weakly T-dependent

Outline

1. Empirical observations regarding HCl
2. Hot carrier dissociation of SiH bonds
3. Hot carrier dissociation of SiO bonds
4. Conclusions

Si-O bond dissociation



Degree of heating of the carriers

Dissociation of the bonds

(1) Electrons heated by field

SiH dissociation...

(2) Hot electrons break SiH bonds

SiO dissociation...

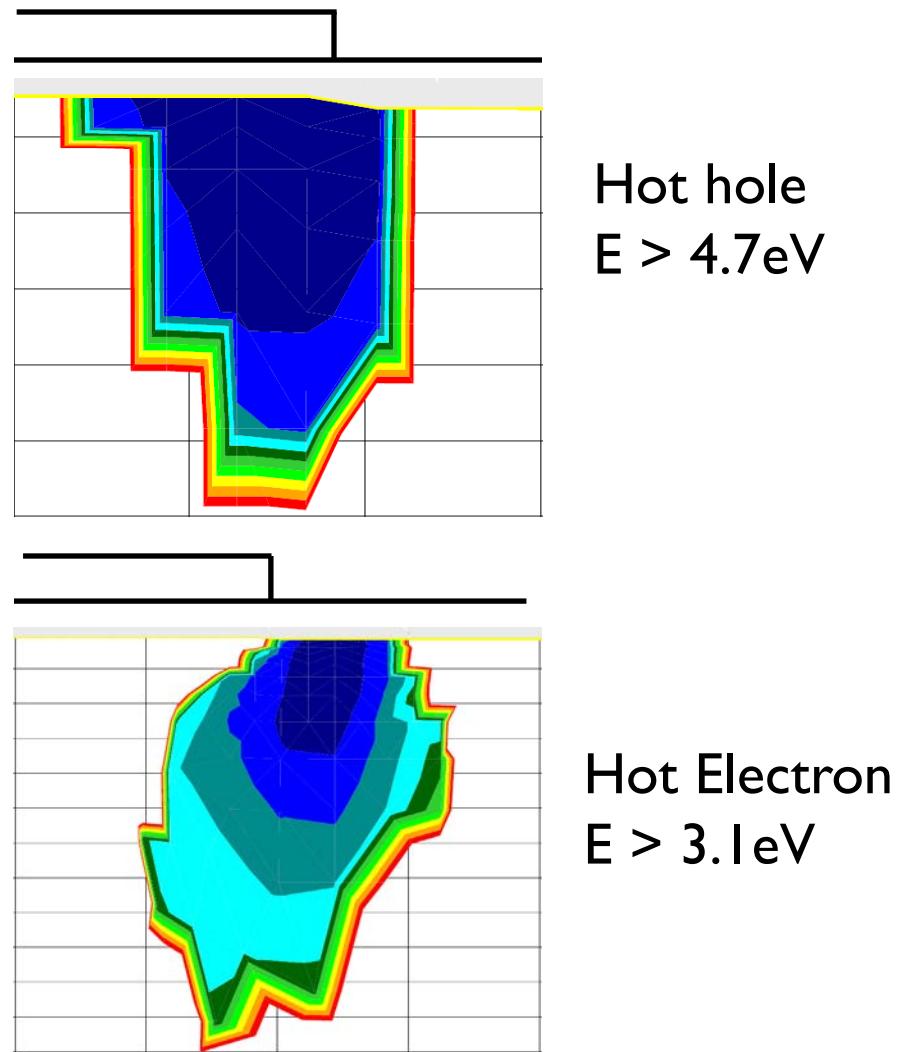
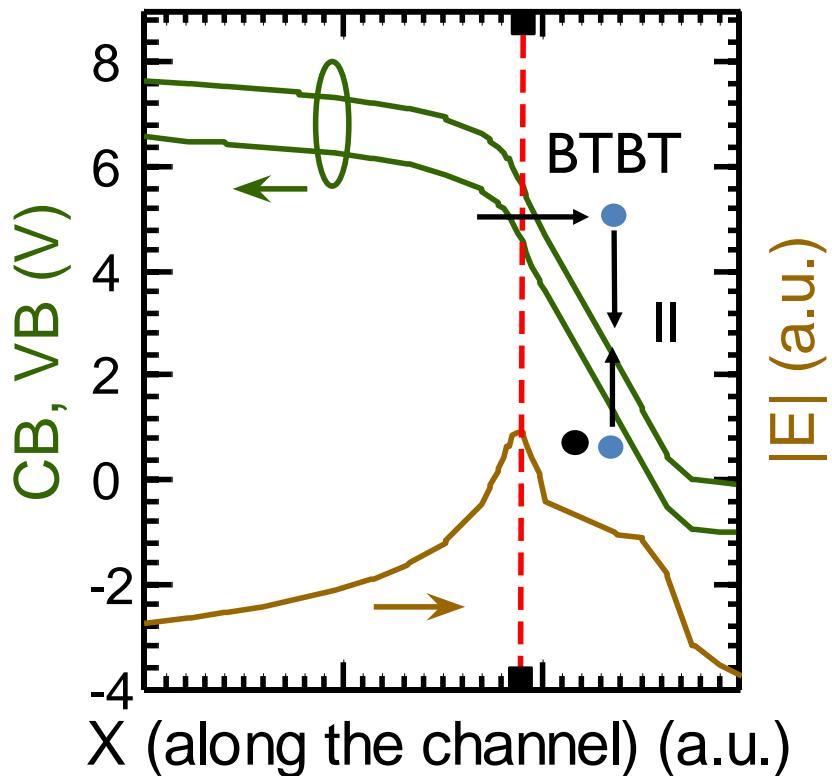
(3) Hot electron produces

Hot holes through II

Hot holes break SiO bonds

Explore the T-dependencies of both

Recall: Heating of Electrons



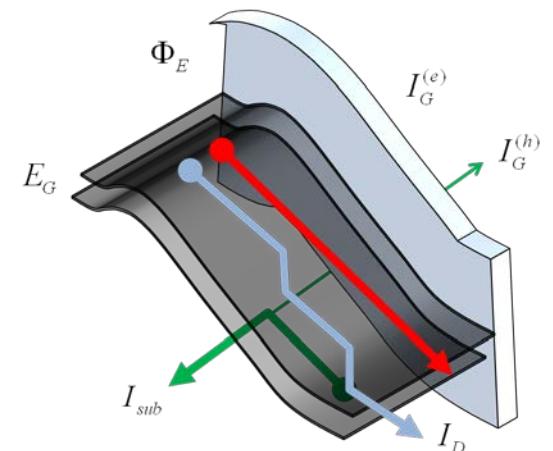
Impact Ionization by the hot electrons generate hot holes

Temp dependence of impact ionization

$$I_{sub} = \int_0^l I_e(x) \times S_{ii} dx .$$

$$= \int_0^l dx \int_0^\infty dE \times qn_0 \left(\frac{k_B T_e(x)}{2\pi m^*} \right)^{1/2} e^{\frac{-E}{k_B T_e(x)}} \times S_{ii}(E > E_T)$$

$$= \int_0^l dx qn_0 \left(\frac{k_B T_e(x)}{2\pi m^*} \right)^{1/2} \int_{\Phi_{ii}}^\infty dE e^{\frac{-E}{\mathcal{E}_m \lambda_e}} \times S_{ii}(E > E_T)$$



‘Hot’ electrons cooler at higher lattice temperature,
because mean-free path is smaller.

Recall: Rate of impact ionization

For $E > \Phi_{ii}$

$$S_{ii} \approx C_{ii} \left[\left(E/\Phi_{ii} \right) - 1 \right]^\gamma$$

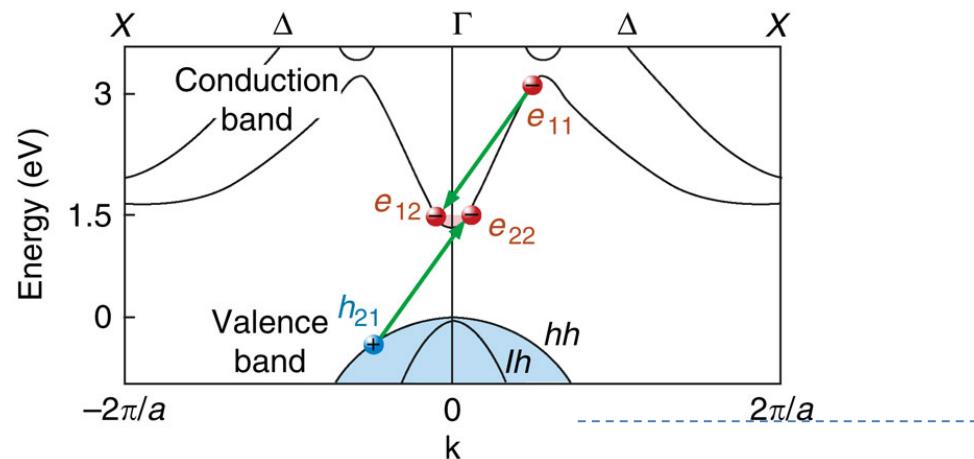
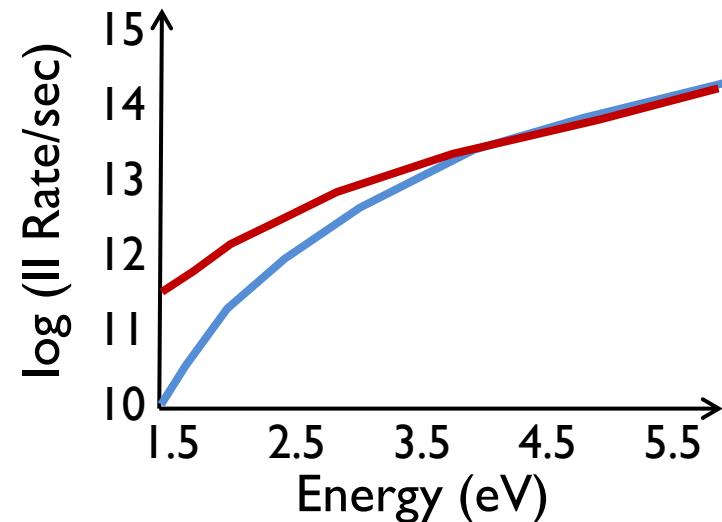
$$\Phi_{ii} \approx E_G(T_L) \left(1 + \frac{m_e}{m_e + m_h} \right)$$

$$\Phi_{ii} = 1.75 \text{ eV},$$

$$C_{ii} = 10^{12} \text{ s}^{-1},$$

$$\gamma = 1$$

$$m = 0.5m_0$$



Temp. Dependence of Impact ionization

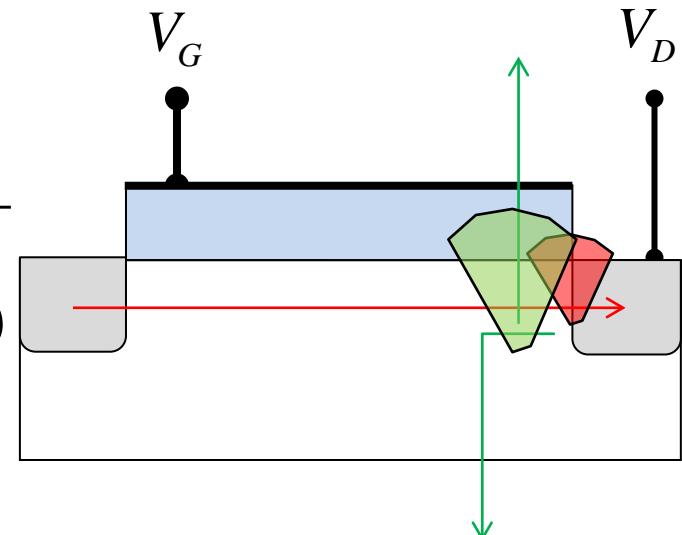
$$\frac{I_{sub}(T_L)}{I_{sub}(T_{L,ref})} = \frac{\int_{\Phi_{ii}}^{\infty} dE e^{\frac{-E}{\epsilon_m \lambda_e(T_L)}} S_{ii}(E > E_T)}{\int_{\Phi_{ii}}^{\infty} dE e^{\frac{-E}{\epsilon_m \lambda_e(T_{L,ref})}} S_{ii}(E > E_T)}$$

$$\approx \frac{e^{\frac{-\Phi_{ii}}{\epsilon_m \lambda_e(T_L)}}}{e^{\frac{-\Phi_{ii}}{\epsilon_m \lambda_e(T_{L,Ref})}}} \left[\frac{k_B T_L}{k_B T_{L,Ref}} \right]^\gamma$$

$$\square e^{\frac{-\Phi_{ii}}{\epsilon_m} \left[\frac{1}{\lambda_e(T_L)} - \frac{1}{\lambda_e(T_{L,Ref})} \right]}$$

With $\frac{\lambda_e(T_L)}{\lambda_e(T_{ref})} = \left[\frac{2n_{ph}(T_{ref}) + 1}{2n_{ph}(T_L) + 1} \right]$

$$n_{ph}(T) \equiv [\exp(\hbar\omega/k_B T_L) - 1]^{-1}$$



Impact ionization suppressed at higher T,
so is the hot hole population

T-Dependent SiO dissociation: RRK Theory

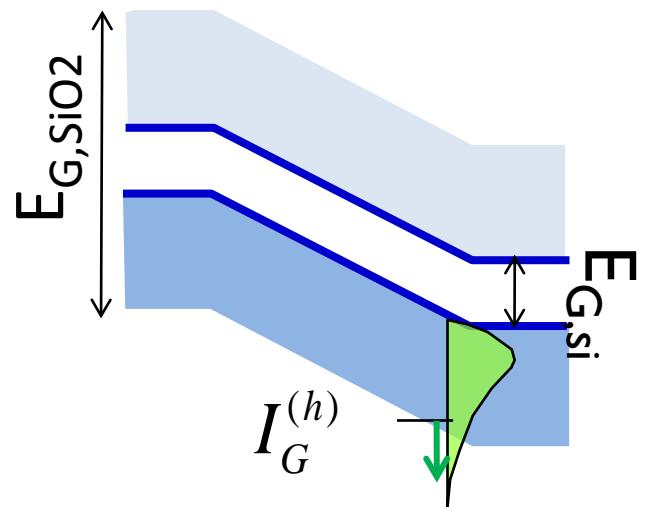
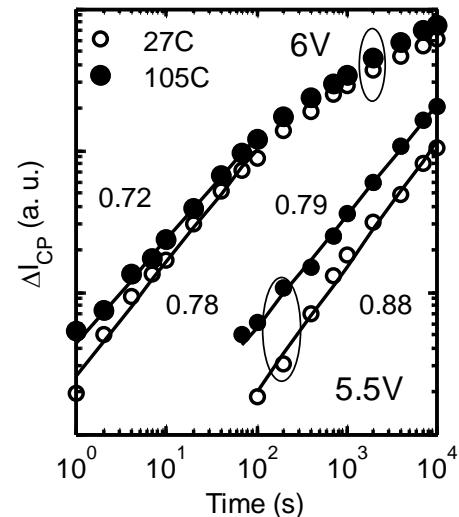
$$N_{IT,SiO} = \sum_E g(E) \left[1 + e^{-k_F(V_G, V_D)t} \right] dE$$

$$k_F \propto I_h \times e^{-\Phi_h/\epsilon_m \lambda_h} \times F_{sio}$$

$$I_h(T_L) \square I_h(T_{L,\text{ref}}) e^{\frac{-\Phi_{ii}}{\epsilon_m} \left[\frac{1}{\lambda_e(T_L)} - \frac{1}{\lambda_e(T_{L,\text{Ref}})} \right]}$$

↓

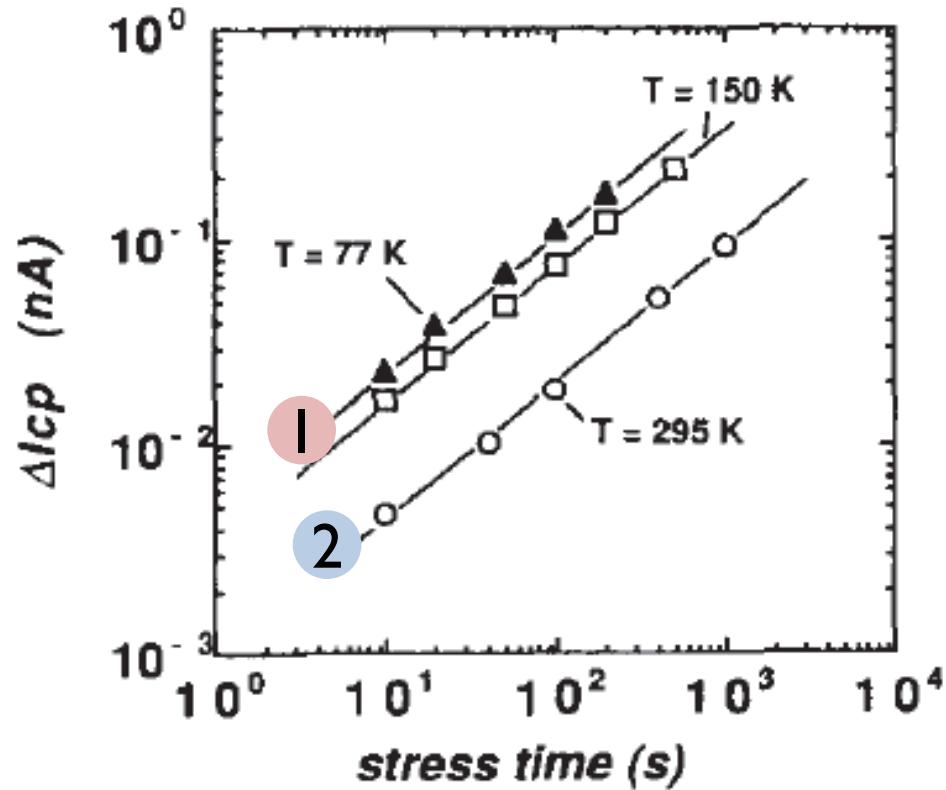
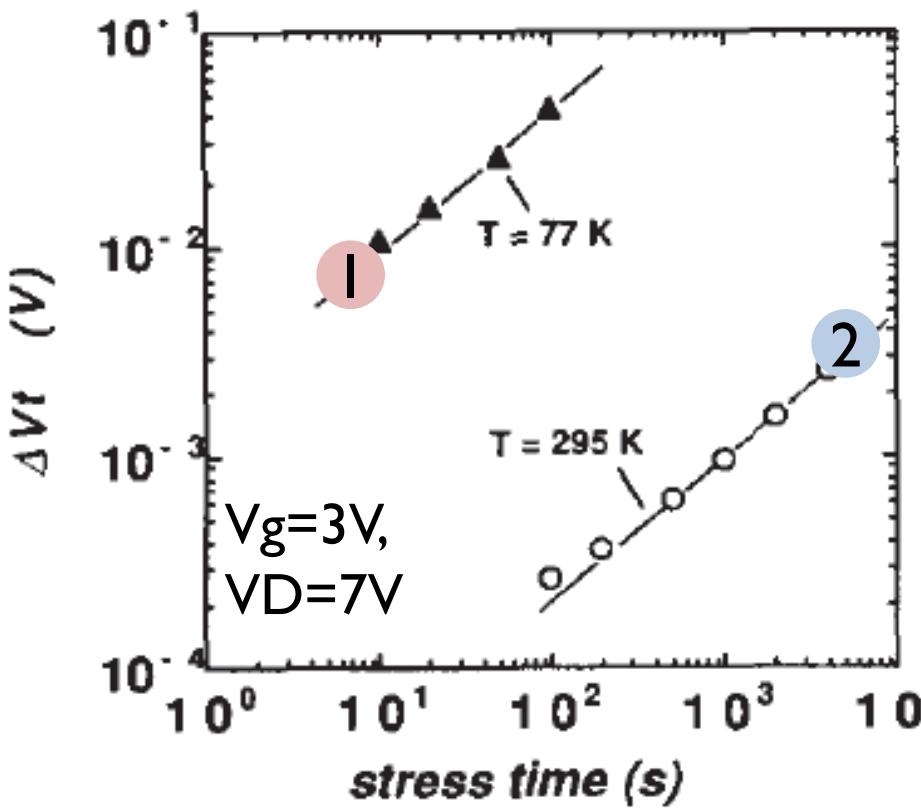
$$k_F^{(\text{HCl})} \propto \left(\frac{e^{\frac{(E_F - \Delta E_{I_G})}{kT_L}}}{\Gamma_E(T_L)} \uparrow \right) \uparrow \downarrow \quad \left(\Gamma_E^{(0)} \right) = B e^{DT_L}$$



SiO barrier larger, could be fully compensated

If compensated, what about VT shift?

P. Heremans, TED, 37(4), p. 980, 1990.

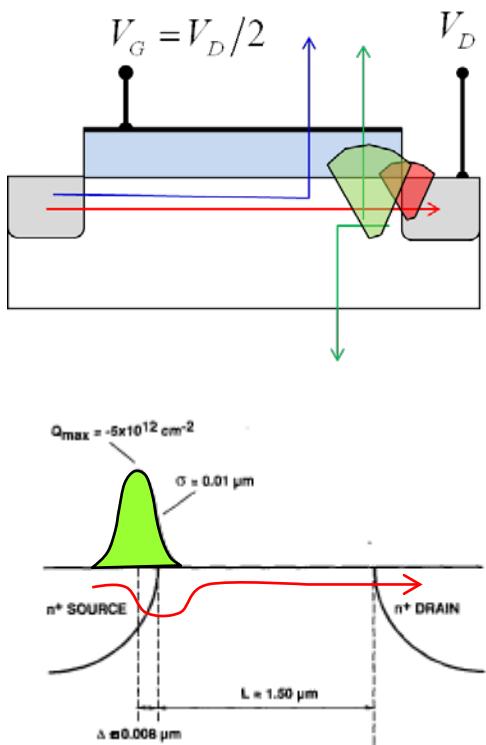


Less degradation at higher temperature

$I_{cp} \sim N_{it}$ and Not confirms trap generation

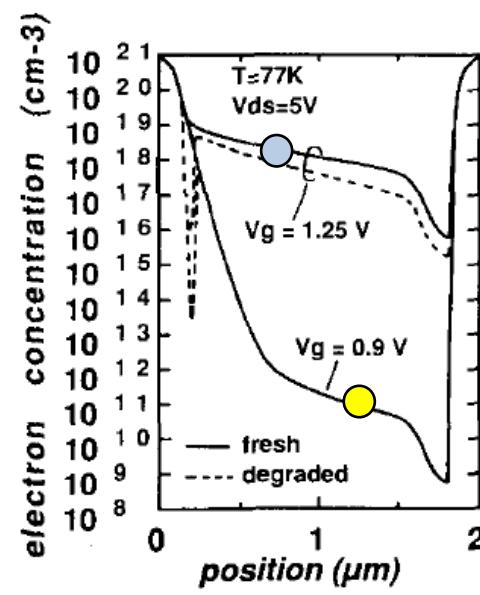
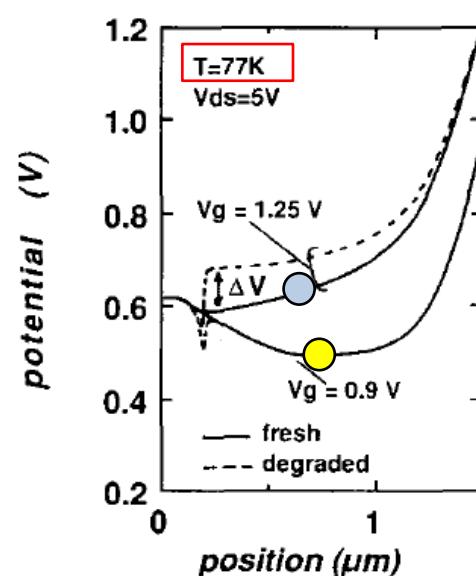
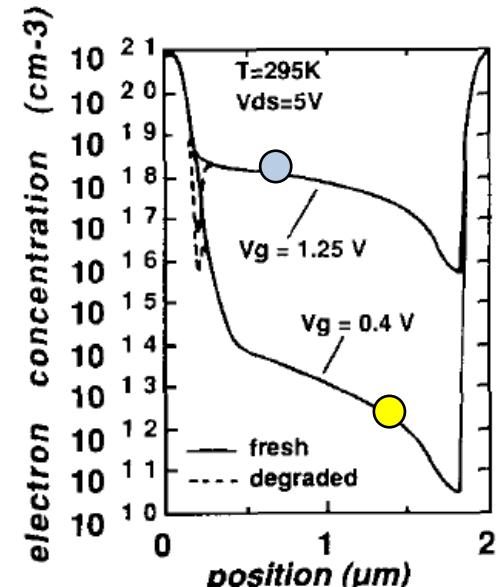
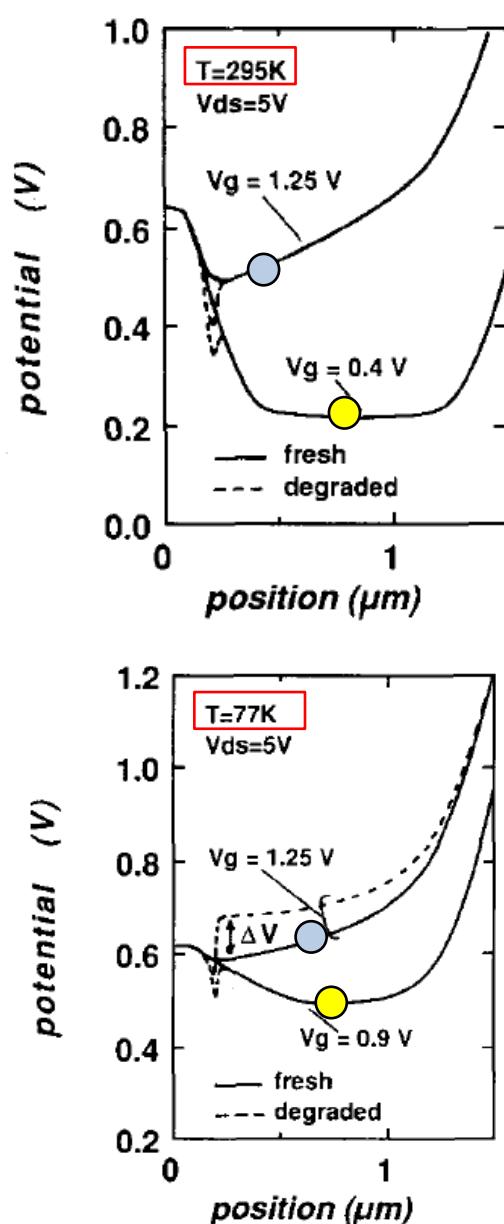
After dE correction, N_{it} could be larger at higher temperature

The puzzle of VT shift



Relative barrier height is larger at smaller temperature

P. Heremans, TED, 37(4), p. 980, 1990.



Conclusions

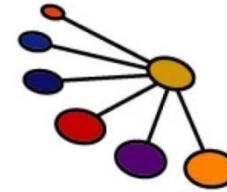
- 1) HCl temperature dependence is pronounced for VT at lower temperature. The defect generation – as reflected in CP signal – is essentially temperature independent.
- 2) In general, it is more difficult to meet VT-based HCl lifetime requirement at lower temperature.
- 3) Two different theories could explain the temperature dependence of HCl – MVE and RRK theories.
- 4) HCl measurement allows a unique probe to the status of carriers within the devices and have often been used as a calibration tool for device modeling.
- 5) HCl based writing is the key to all Flash memories.

References

- Much of the original work on HCl is summarized in C. Hu et al., IEEE Trans. Elec. Dev. ED-32, 375, 1985; S. Tam, P. Ko, and C. Hu, IEEE Trans. Elec. Dev. ED-31, 1116, 1984.
- Theory of Si-H bond dissociation was developed by K. Hess et al, Physica E, 3, 1, 1997. Ph. Avouris *et al*, Chem. Phys. Lett., 257, 148, 1996. Also see K. Hess, Giant Isotope effect in HCD of Metal oxide Silicon Devices, 45(2), 406, 1998.
- The theory of Multiple Vibrational Excitation is discussed in T.-C. Shen, C. Wang, G. C. Abeln, J. R. Tucker, J. W. Lyding, Ph. Avouris, and R. E. Walkup, "Atomic-scale desorption through electronic and vibrational excitation mechanisms", *Science*, vol. 268, pp.1590 1995. The RRK theory is discussed by Kimerling, SSE, 21(11), 1978.
- J. Bude, 'Gate current by II feedback in sub-micron technologies', VLSI Proc. p. 101-102, 1995. developed MC models for more accurate description of the distribution function.
- R. Bellens, P. Heremans, G. Grosenekan, and H. E. Maes, IRPS 1988.
- A very comprehensive theory of HCl can be found in the 2010 Thesis by D. Varghese, Purdue University. A theory of time exponent for SiH bond dissociation can be found in H. Kulfuoglu, Journ. Comput. Electron., 3, 165, 2004.
- The electron-holes recombination theory is due to L.C. Kimberly discussed in "Recombination enhanced defect reactions", Solid State Electronics, 21(11), 1978.
- Negative temperature activation is discussed in Lifetimes of Hydrogen and Deuterium Related Vibrational Modes in Silicon M. Budde, PRL, 87(14), 2001.
- IEEE TRANSACTIONS ON ELECTRON DEVICES. VOL. 37. NO 4.APRIL 1990, p. 980.Temperature dependence of the channel hot-carrier degradation of n-channel mosfet's, PAUL HEREMANS, GEERT VAN DEN BOSCH, RUDI BELLENS, GUIDO GROESENEKEN.

Self Test Review questions

1. What is the difference between hot atom dissociation vs. cold atom dissociation?
2. Many experiments are reported at 77K and 295K. Why these temperatures?
3. Why is there such a big difference between VT degradation and NIT degradation?
4. Impact ionization threshold is significantly larger than Eg. What role does it have for HCl degradation? Explain.
5. Will there be no HCl degradation if VD reduced below impact ionization threshold? What theory would you use to calculate the defect generation rate.



ECE695: Reliability Physics of Nano-Transistors

Lecture 16: Appendices

Temperature dependence of HCI

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Appendices

1. Equilibrium theory of forward and reverse dissociation
2. Rice-Ramsperger-Kassel Theory of bond dissociation
3. Multi-vibration Coherent Excitation Theory of Bond dissociation
4. Conclusion

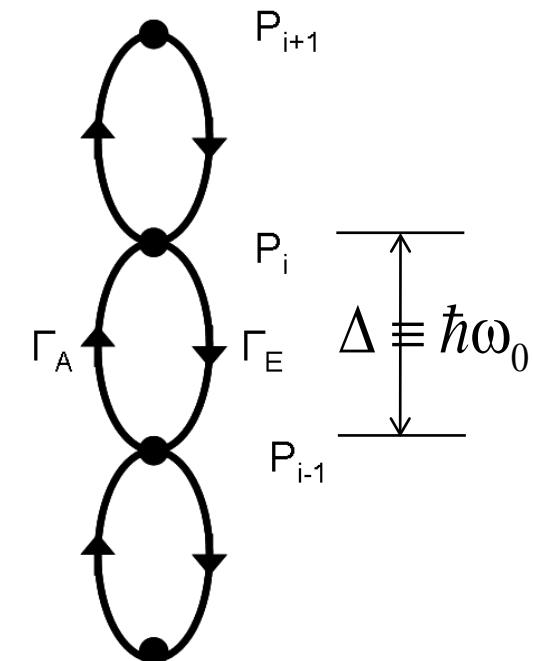
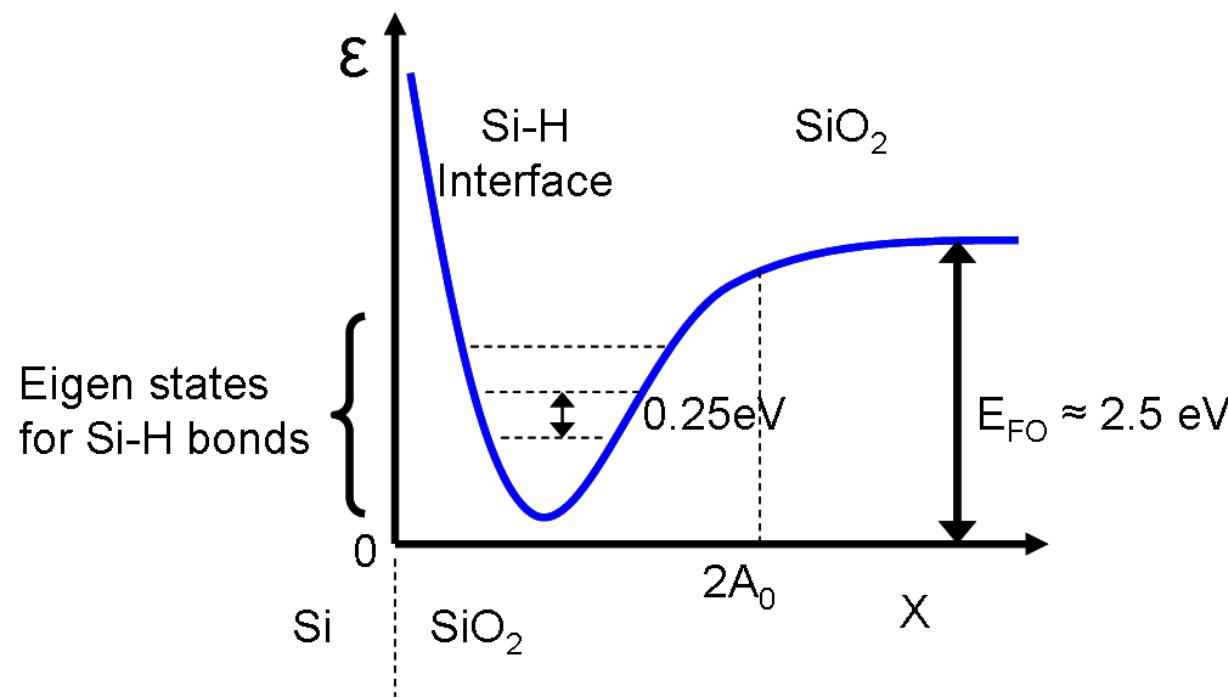
Appendix 1: T-dependence of k_F and k_R

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

$$F = \Gamma_0 (n_{\max} + 1) \times \left[\frac{\Gamma_{ext}}{\Gamma_{ext} + \Gamma_0} \right]^{n_{\max} + 1}$$

$$n_{\max} \equiv \frac{E_F}{\hbar\omega_0} = \frac{E_F}{\Delta}$$

Consider an harmonic oscillator with equally spaced levels ...



Transition rates due to phonons

In a harmonic oscillator ...

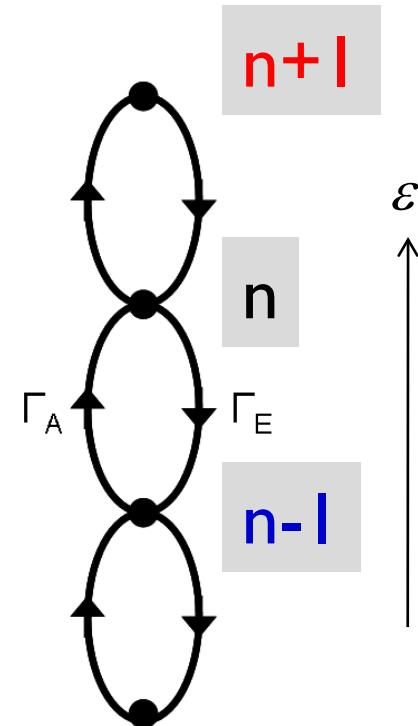
$$A u_n = \sqrt{n} u_{n-1}$$

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

Therefore the transition rate is ...

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

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



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

Absorbing/Emitting phonons in Equilibrium

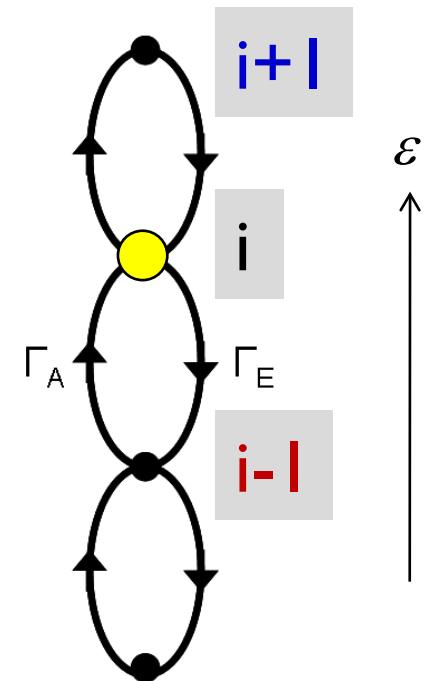
Probability of a Si-H bond at the i-th vibration mode ...

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

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

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

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



Absorbing/Emitting phonons in Equilibrium

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

Detailed balance ...

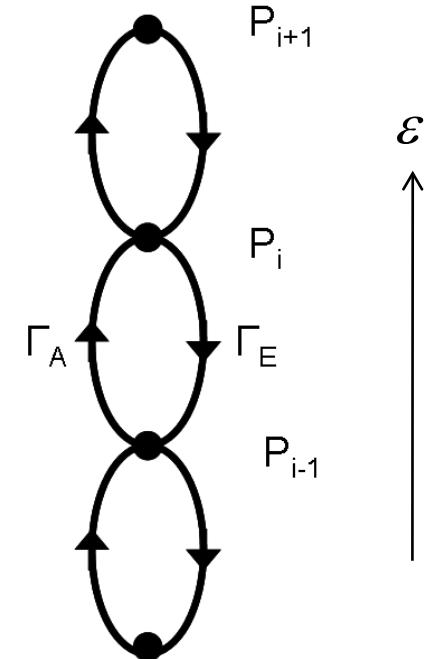
$$\left. \begin{aligned} \frac{\Gamma_A}{\Gamma_E} &= e^{-\Delta/k_B T} \approx 1 - \frac{\Delta}{k_B T} \\ \frac{\Gamma_A}{\Gamma_E} &= \frac{\Gamma_0(1-\delta/2)}{\Gamma_0(1+\delta/2)} = 1 - \delta \end{aligned} \right\} \quad \delta = \frac{\Delta}{k_B T}$$

$$P(\varepsilon_i) = C \times e^{-\varepsilon_i/k_B T}$$

and C by normalization

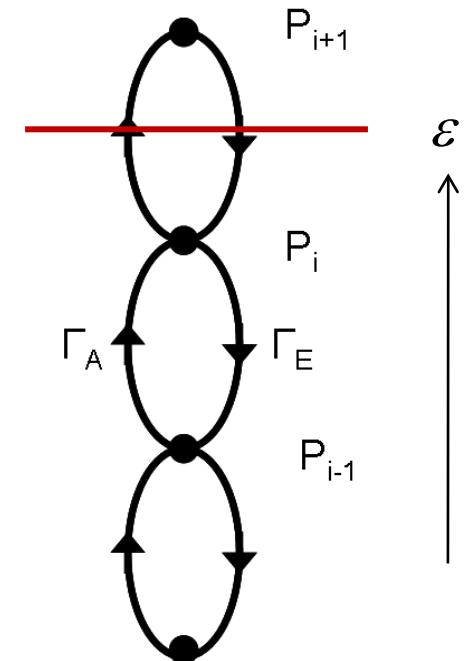
$$\sum_i p(\varepsilon_i) = 1$$

Approximate Bose-Einstein distribution



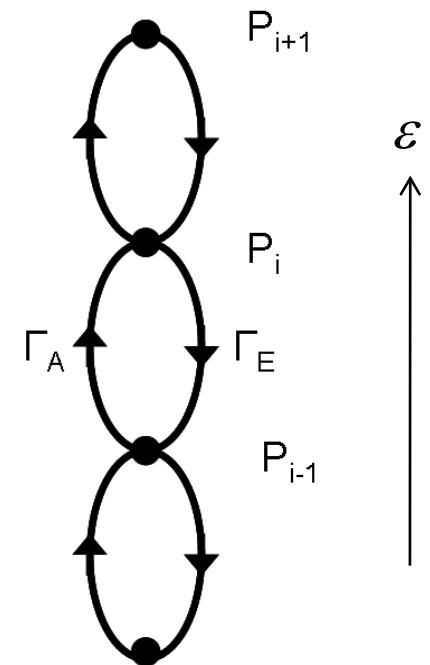
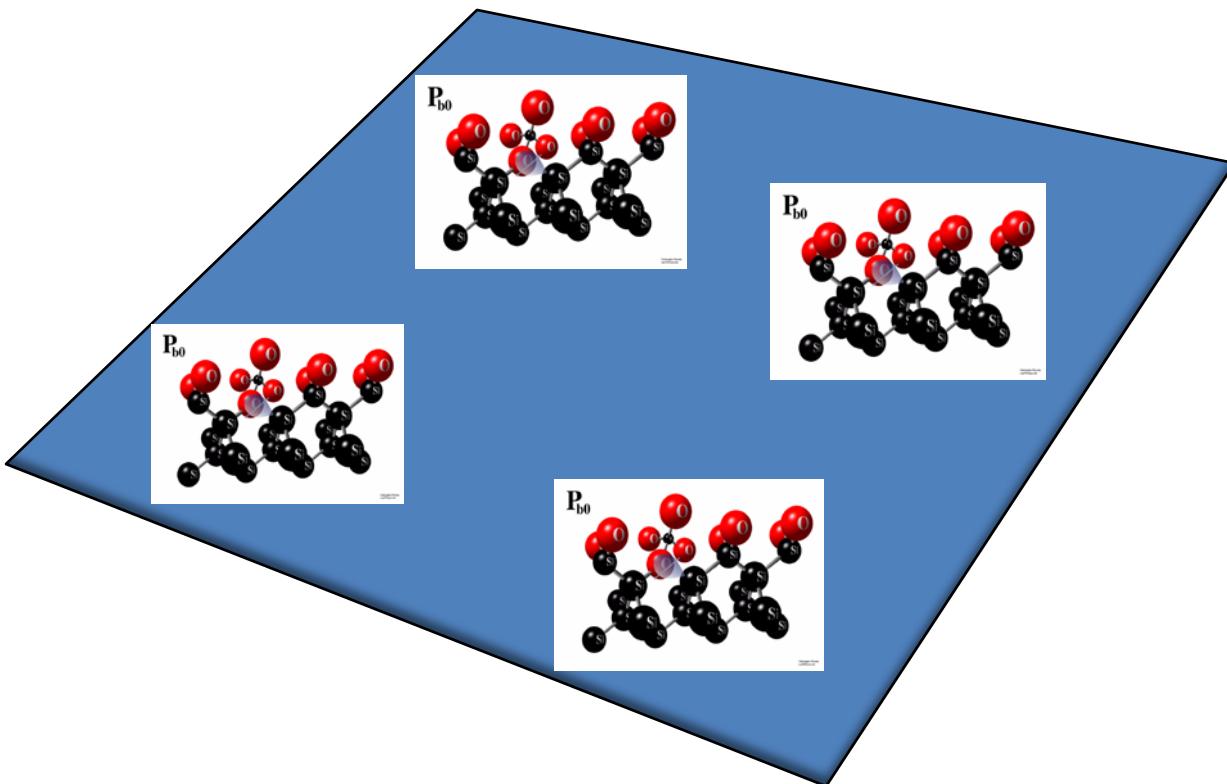
Net flux in Equilibrium

$$\begin{aligned} F &= (i+1)\Gamma_A P_i - i\Gamma_E P_{i+1} \\ &= (i+1)\Gamma_A P_i \left(1 - \frac{\Gamma_E}{\Gamma_A} \frac{P_{i+1}}{P_i}\right) \\ &= (i+1) \times \Gamma_A P_i \left(1 - e^{\frac{\Delta}{k_B T}} \frac{e^{-\frac{\Delta \times (i+1)}{k_B T}}}{e^{-\frac{\Delta \times (i)}{k_B T}}}\right) = 0 \end{aligned}$$



... as expected.

Meaning of the distribution ...



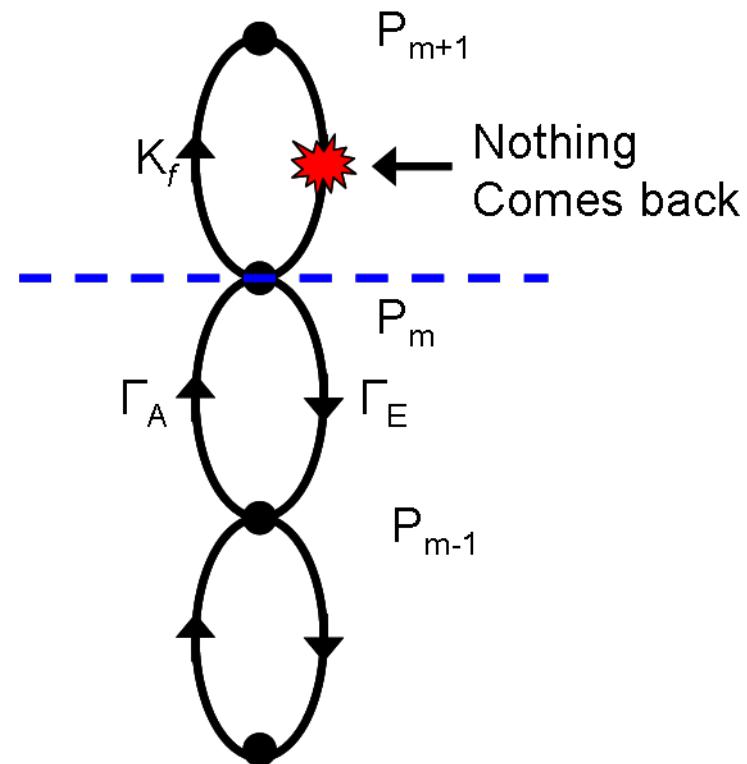
Interpretation

Probability that a Si-H climbs the barrier

... that it finally absorbs a phonon to break the bond

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

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



Appendix 2: Hot carrier induced dissociation by MVE (Coherent)

In thermal equilibrium ...

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

Rates with injected current ...

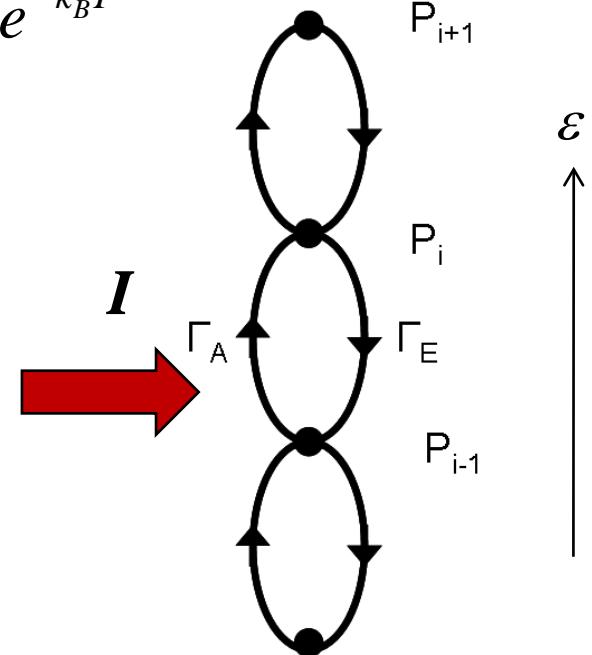
$$\Gamma_A = \Gamma_A^{(0)} + (I/q) f_{in} \quad \Gamma_E = \Gamma_E^{(0)} + (I/q) f_{in}$$

Dissociation rates of Si-H bonds ...

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

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

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



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 ...

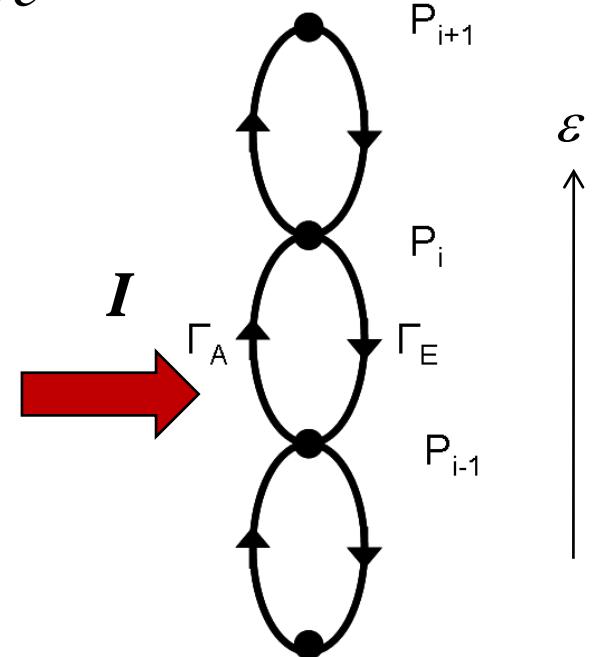
$$\Gamma_A = \Gamma_A^{(0)} + (I/q) f_{in} \quad \Gamma_E = \Gamma_E^{(0)} + (I/q) f_{in}$$

Dissociation rates of Si-H bonds ...

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

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

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



Salam, PRB, 1994.

Appendix 3: Derivation of the RRK Model

Show that the occupation of level i for a molecule with s -degrees of freedom in equilibrium is given by ...

$$P_{i,0} \sim \frac{1}{(s-1)!} \left(\frac{E}{kT} \right)^{s-1} \frac{e^{-E_i/k_B T}}{kT}$$

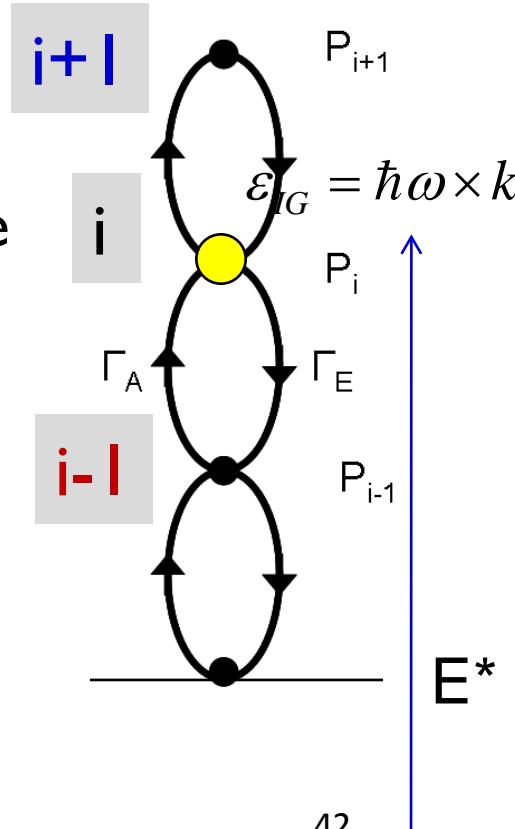
And that any one of the atom within the molecule will get energy more than E^* is given by the DOS

$$D(E) = (E - E^*) / E^{s-1}$$

So that the enhanced dissociation is given by

$$F_{IG} \propto \frac{m(I_G f_i/q)}{(\Gamma_A + \Gamma_E)} \left(\frac{E^* - E_{IG}}{E^*} \right)^{s-1} \times e^{-(E^* - E_{IG}/kT)}$$

Alam ECE 695



Dissociation with an energy kick

Probability of a Si-H bond at the **i-th** vibration mode with kick ...

$$i\Gamma_A P_{i-1} + (i+1)\Gamma_E P_{i+1} - (i+1)\Gamma_A P_i - i\Gamma_E P_i + (I_G f_i/q)P_{i-k} = 0$$

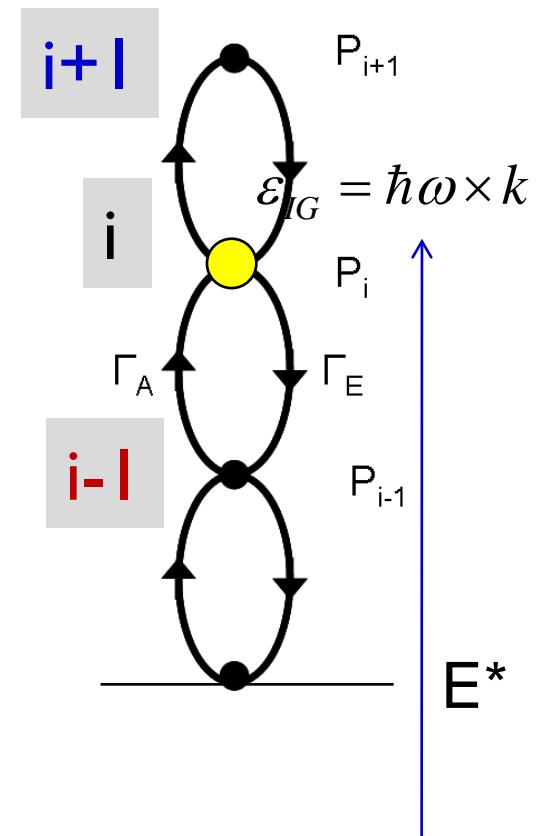
Solve for **i-th state ..**

$$P_i = \frac{i}{(\Gamma_A + \Gamma_E)} (\Gamma_E P_{i+1} + \Gamma_A P_{i-1}) + \frac{i P_{i-k}}{(\Gamma_A + \Gamma_E)} (I_G f_i/q)$$

$$\text{For } s=1, P_{i,0} = \frac{e^{-E_i/k_B T}}{kT} \text{ (See L11)}$$

$$\text{For } s>1 P_{i,0} \sim \frac{1}{(s-1)!} \left(\frac{E}{kT} \right)^{s-1} \frac{e^{-i\Delta/k_B T}}{kT}$$

Will now be shown



Distribution function with internal degree of freedom (e.g. two atoms, S=1)

$$\text{For } s>1 \quad P_{i,0} \sim \frac{1}{(s-1)!} \left(\frac{E}{kT} \right)^{s-1} \frac{e^{-i\Delta/k_B T}}{kT}$$

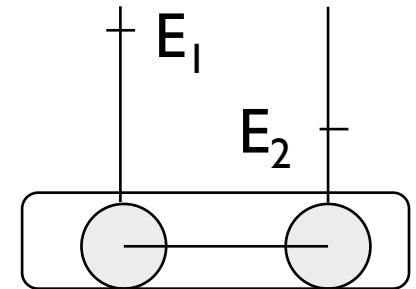
$$f(E) = \frac{e^{-E/k_B T}}{kT} dE$$

$$f(E = E_1 + E_2) = f(E_1)f(E_2) = \left(\frac{1}{kT} \right)^2 e^{-E/k_B T} dE_1 dE_2$$

$$f(E_A \leq E \leq E_B) = f(0 \leq E \leq E_B) - f(0 \leq E \leq E_A)$$

$$f(0 \leq E \leq E_A) = \left(\frac{1}{kT} \right)^2 e^{-E/k_B T} \int_0^{E_A} dE_1 \int_0^{E_A - E_1} dE_2$$

$$= \left(\frac{1}{kT} \right)^2 e^{-E/k_B T} \frac{E_A^2}{2!}$$



Dissociation with an energy kick

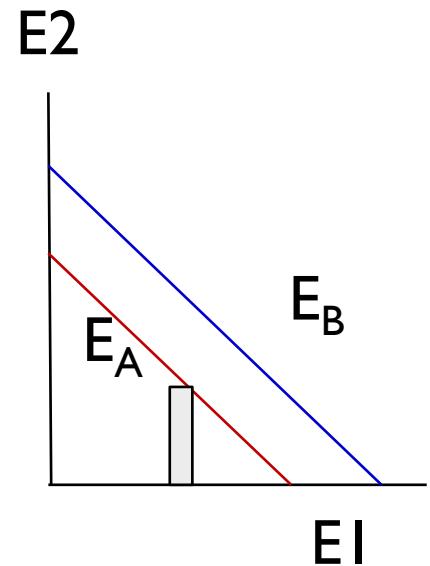
Continuing after the previous page ...

$$f(E_A \leq E \leq E_B) = f(0 \leq E \leq E_B) - f(0 \leq E \leq E_A)$$

$$= \left(\frac{1}{kT} \right)^2 e^{-E/k_B T} \left(\frac{E_B^2}{2!} - \frac{E_A^2}{2!} \right)$$

$$= \left(\frac{1}{kT} \right)^2 e^{-E/k_B T} \left(\frac{(E_A + dE)^2}{2!} - \frac{E_A^2}{2!} \right)$$

$$= \left(\frac{1}{kT} \right)^1 e^{-E/k_B T} \frac{E_A^1}{1!} \frac{dE}{kT} = \left(\frac{E_A}{kT} \right)^{s-1} e^{-E_A/k_B T} \frac{1}{(s-1)!} \frac{dE}{kT}$$



Dissociation with an energy kick

$$P_i = \frac{i}{(\Gamma_A + \Gamma_E)} (\Gamma_E P_{i+1} + \Gamma_A P_{i-1}) + \frac{i P_{i-k}}{(\Gamma_A + \Gamma_E)} (I_G f_i / q)$$

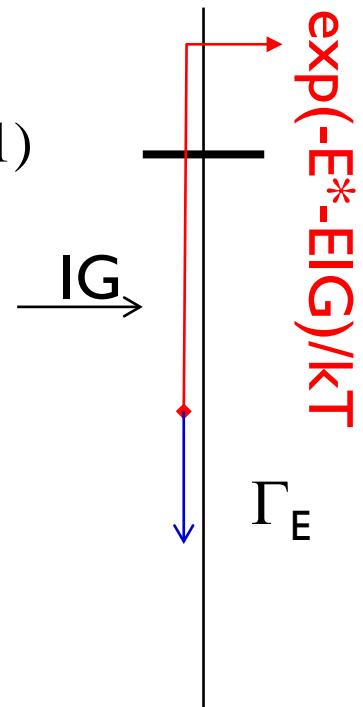
$$\text{Insert } P_{i,0} \sim \frac{1}{(s-1)!} \left(\frac{E}{kT} \right)^{s-1} \frac{e^{-i\Delta/k_B T}}{kT} = \frac{e^{-E_i/k_B T}}{kT} \text{ (if S=1, See L11)}$$

$$F \equiv F_{thermal} + F_{IG} = \sum_{i=m-k}^{\infty} P_s P_i \text{ where } P_s = (E - E^*/E)^{s-1}$$

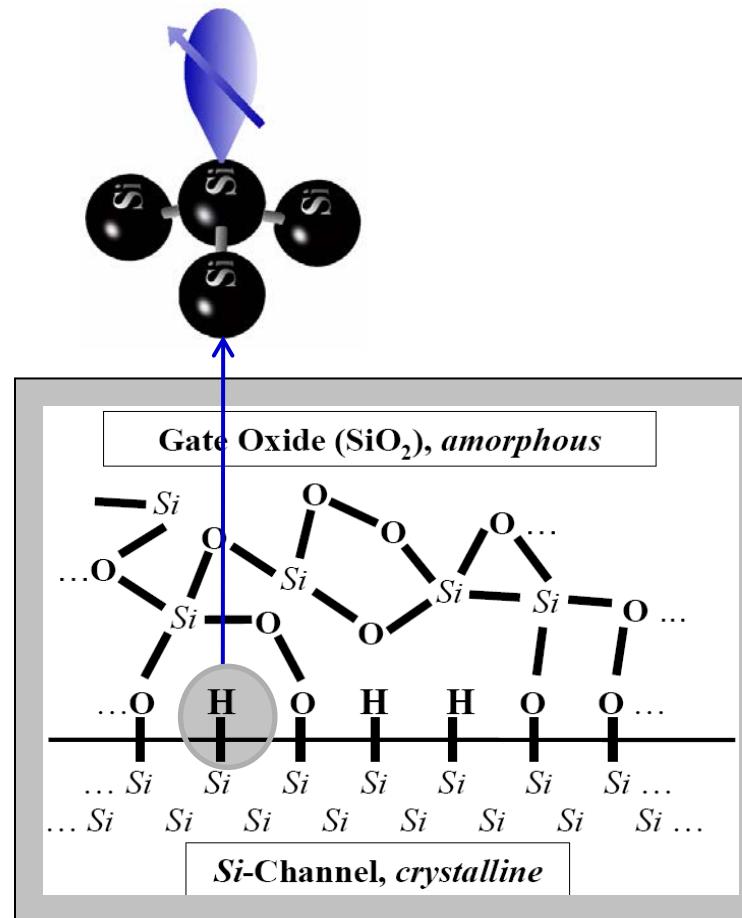
$$F_{IG} \propto \int_{E^*}^{\infty} dE (E - E^*/E)^{s-1} \frac{1}{(s-1)!} \left(\frac{E - E_{IG}}{kT} \right)^{s-1} \frac{e^{-(E - E_{IG})/k_B T}}{kT}$$

$$= \frac{m (I_G f_i / q)}{(\Gamma_A + \Gamma_E)} \left(\frac{E^* - E_{IG}}{E^*} \right)^{s-1} \times e^{-(E^* - E_{IG}/kT)}$$

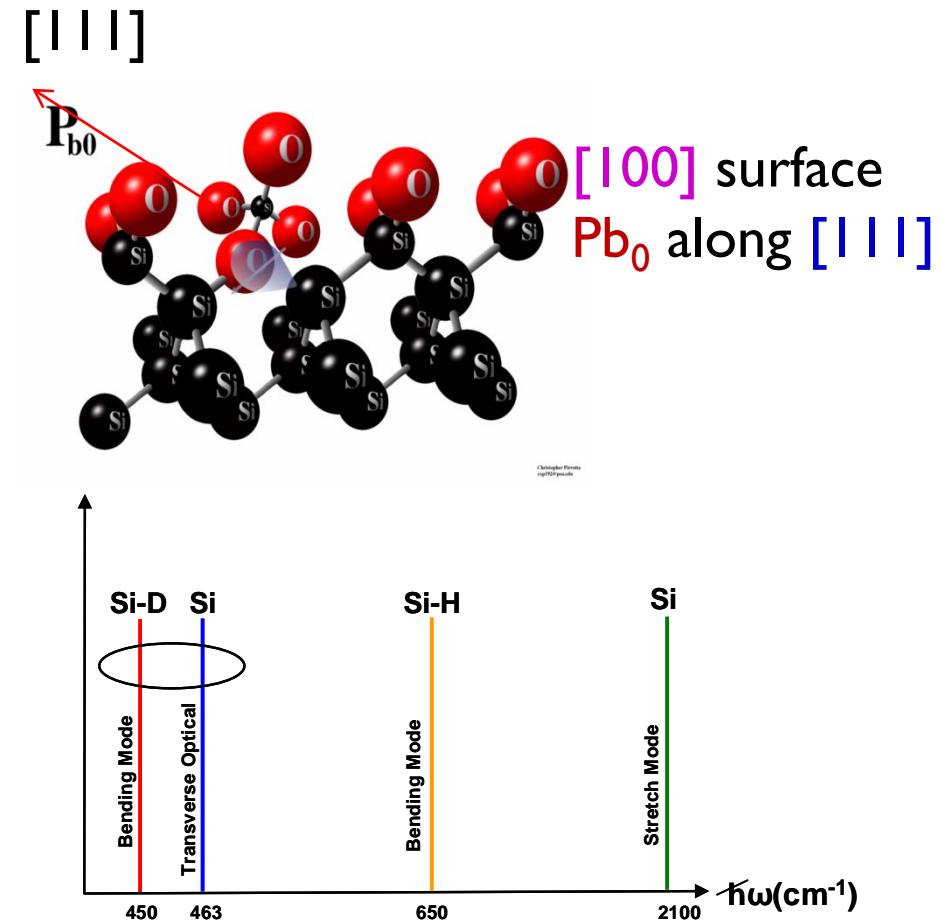
$$\sim \frac{(I_G f_i / q)}{\Gamma_E} \times e^{-(E^* - E_{IG}/kT)} \text{ (for S=1)}$$



Appendix 4: Si-H vs. Si-D bond dissociation



Of Pa, Pb, Pc -- only Pb survives
Related to NBTI degradation



Hydrogen vs. Deuterium Experiments (wrong interpretation through bound levels)

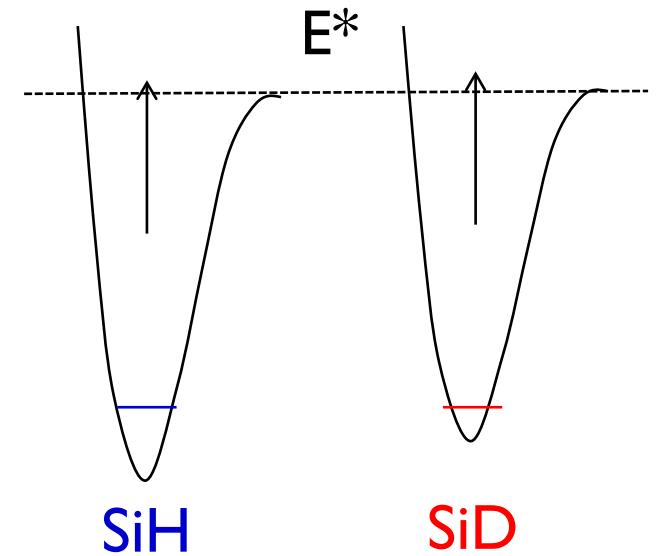
$$F_{IG} \sim \frac{(I_G f_i / q)}{\Gamma_E} \times e^{-(E^* - E_{IG}/kT)} \text{ (for } S=1\text{)}$$

This is wrong

$$F_{IG}^{SiD} \sim \frac{(I_G f_i / q)}{\Gamma_{E,D}} \times e^{-(E_D^* - E_{IG}/kT)}$$

$$F_{IG}^{SiH} \sim \frac{(I_G f_i / q)}{\Gamma_{E,H}} \times e^{-(E_H^* - E_{IG}/kT)}$$

$$\frac{F_{IG}^{SiH}}{F_{IG}^{SiD}} \sim \frac{\Gamma_{E,D}}{\Gamma_{E,H}} \times e^{+(E_D^* - E_H^*)/kT}$$



Mass effect dominant (incorrect)

Phonon coupling to substrate can be neglected (incorrect)

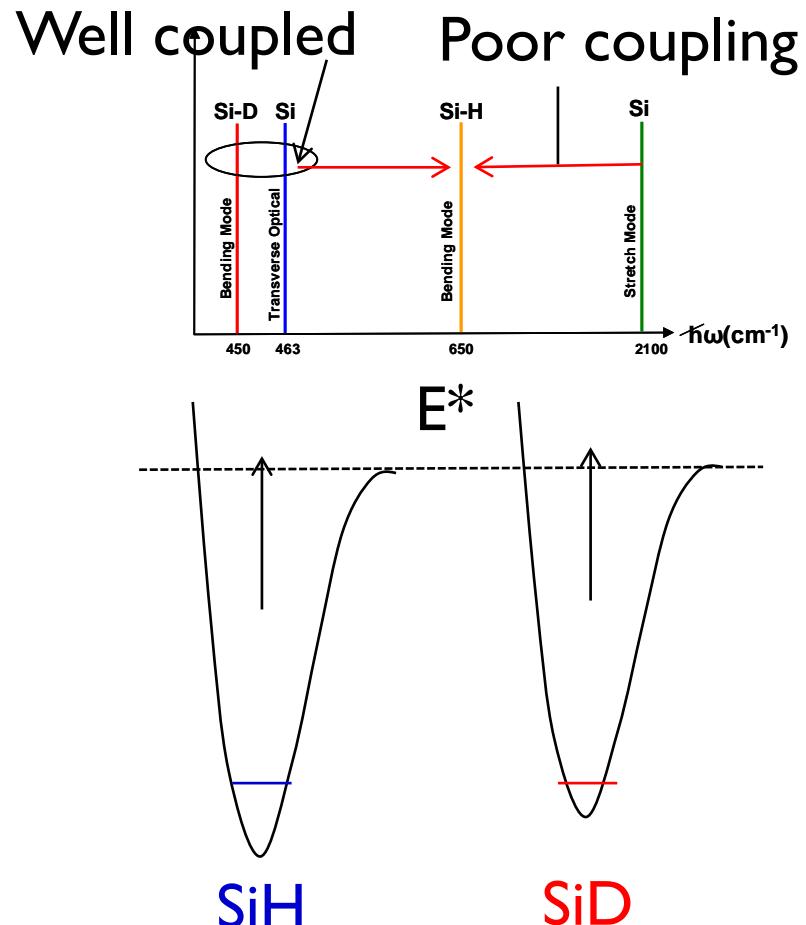
Hydrogen vs. Deuterium Experiments (correct interpretation with phonon coupling)

$$F_{IG} \sim \frac{(I_G f_i / q)}{\Gamma_E} \times e^{-(E^* - E_{IG}/kT)} \text{ (for S=1)}$$

$$F_{IG}^{SiD} \sim \frac{(I_G f_i / q)}{\Gamma_{E,D}} \times e^{-(E^* - E_{IG}/kT)}$$

$$F_{IG}^{SiH} \sim \frac{(I_G f_i / q)}{\Gamma_{E,H}} \times e^{-(E^* - E_{IG}/kT)}$$

$$\frac{F_{IG}^{SiH}}{F_{IG}^{SiD}} \sim \frac{\Gamma_{E,D}}{\Gamma_{E,H}}$$



Phonon coupling to substrate is the dominant cause. SiD better coupled to substrate, so has larger gamma for relaxation.