

# How to Reduce the Dissipation in Glasses

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KITP Electron Glass 2010

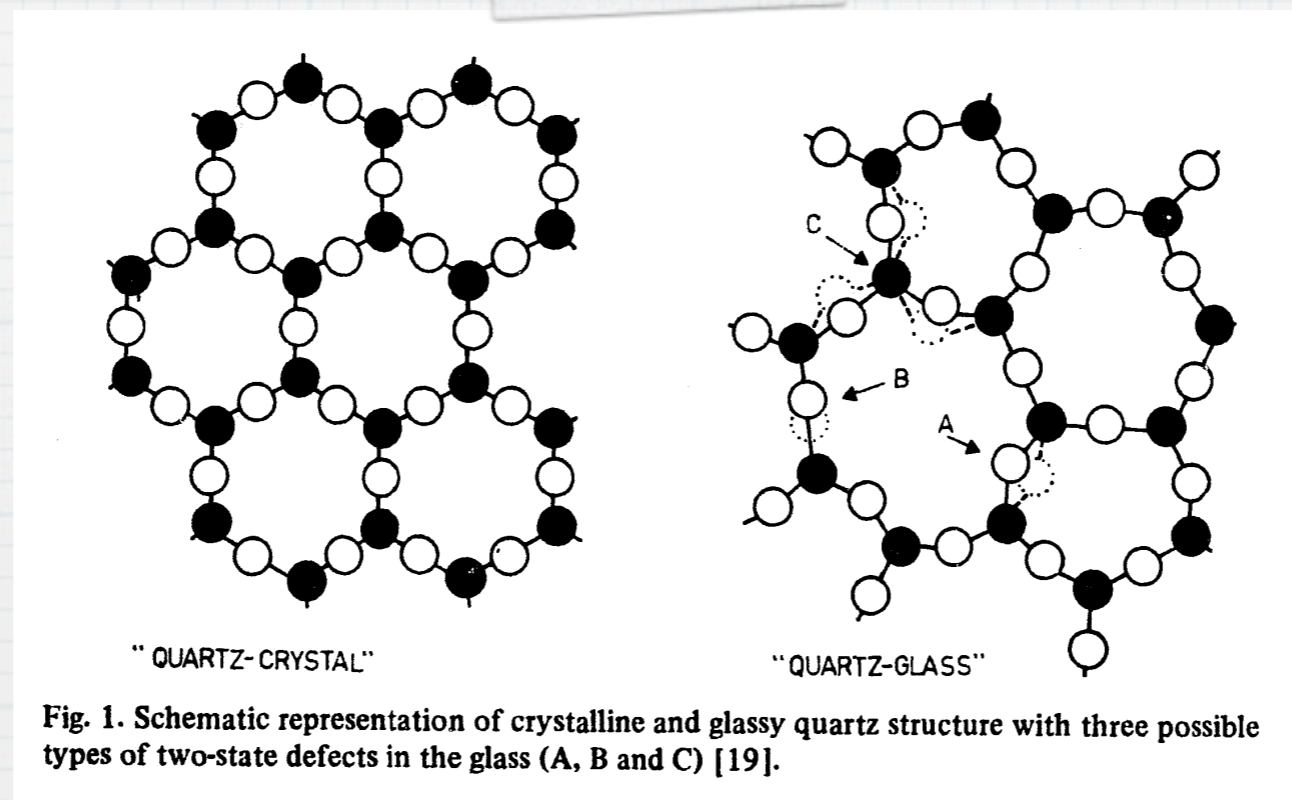
# How to Reduce the Dissipation in Glasses

- \* Introduction to glasses at low temperatures (specific heat, thermal conductivity, two-level-systems model)
- \* Introduction to dissipation in glasses ( how to measure dissipation and theory )
- \* How to reduce acoustic dissipation in glasses (high stress increases barrier heights of defects)
- \* Conclusion

# Introduction to glasses

# Structural glasses

Solids but no long range order



from Jackle, et.al., J.Of.Non-cry. Solid. (1976)

# Specific heat

$$CT^{-3}$$

**Glass**

**Crystals**

Debye theory gives

$$C(T) \propto T^3$$

**Glasses**

Specific heat

- 1) is linear in  $T$  at low temperature
- 2) has peak at 10K

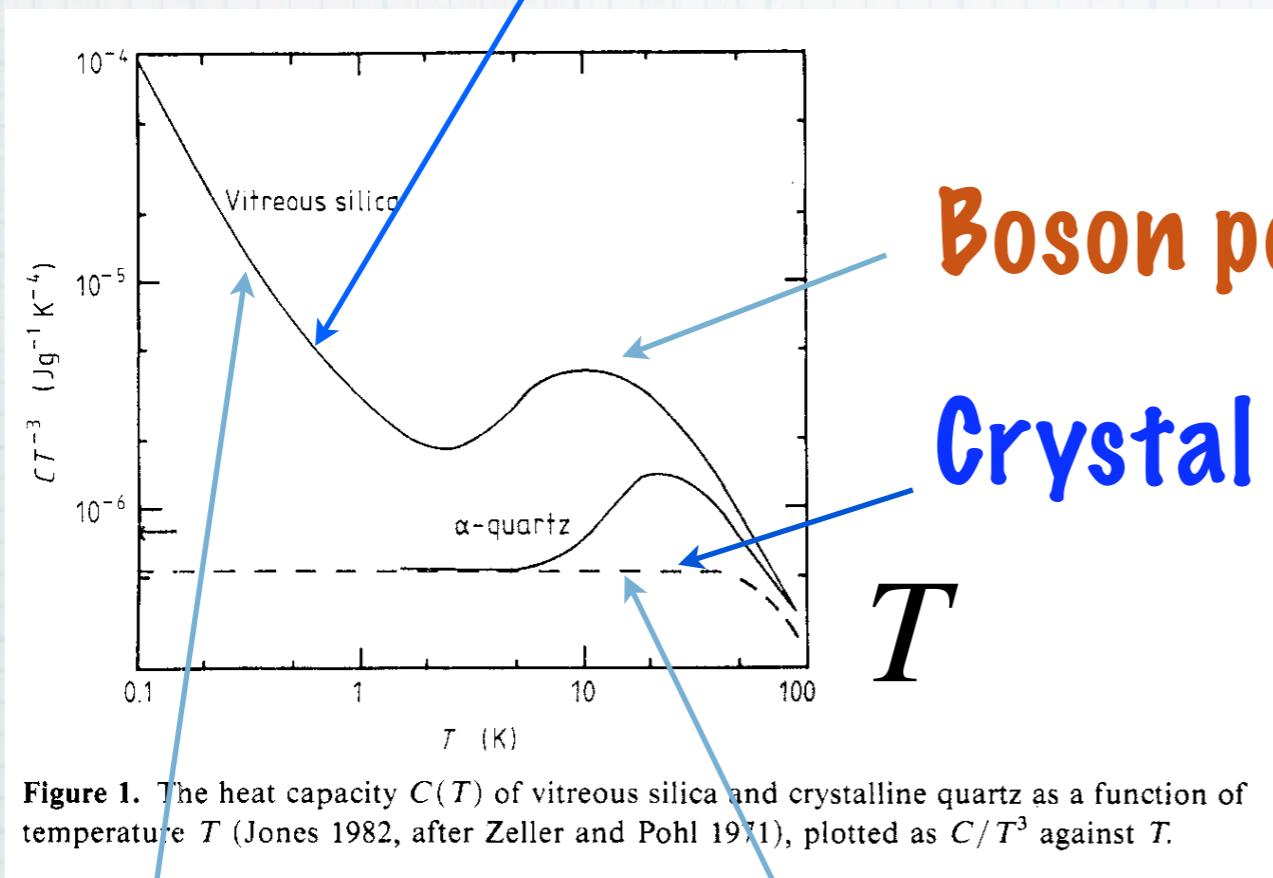


Figure 1. The heat capacity  $C(T)$  of vitreous silica and crystalline quartz as a function of temperature  $T$  (Jones 1982, after Zeller and Pohl 1971), plotted as  $C/T^3$  against  $T$ .

from W.A. Phillips, Rep. Prog. Phys. (1987)

# Linear $T$ term in specific heat

$$C(T) \sim T$$

Zeller and Pohl, (1972)

Seen in a wide variety of glasses

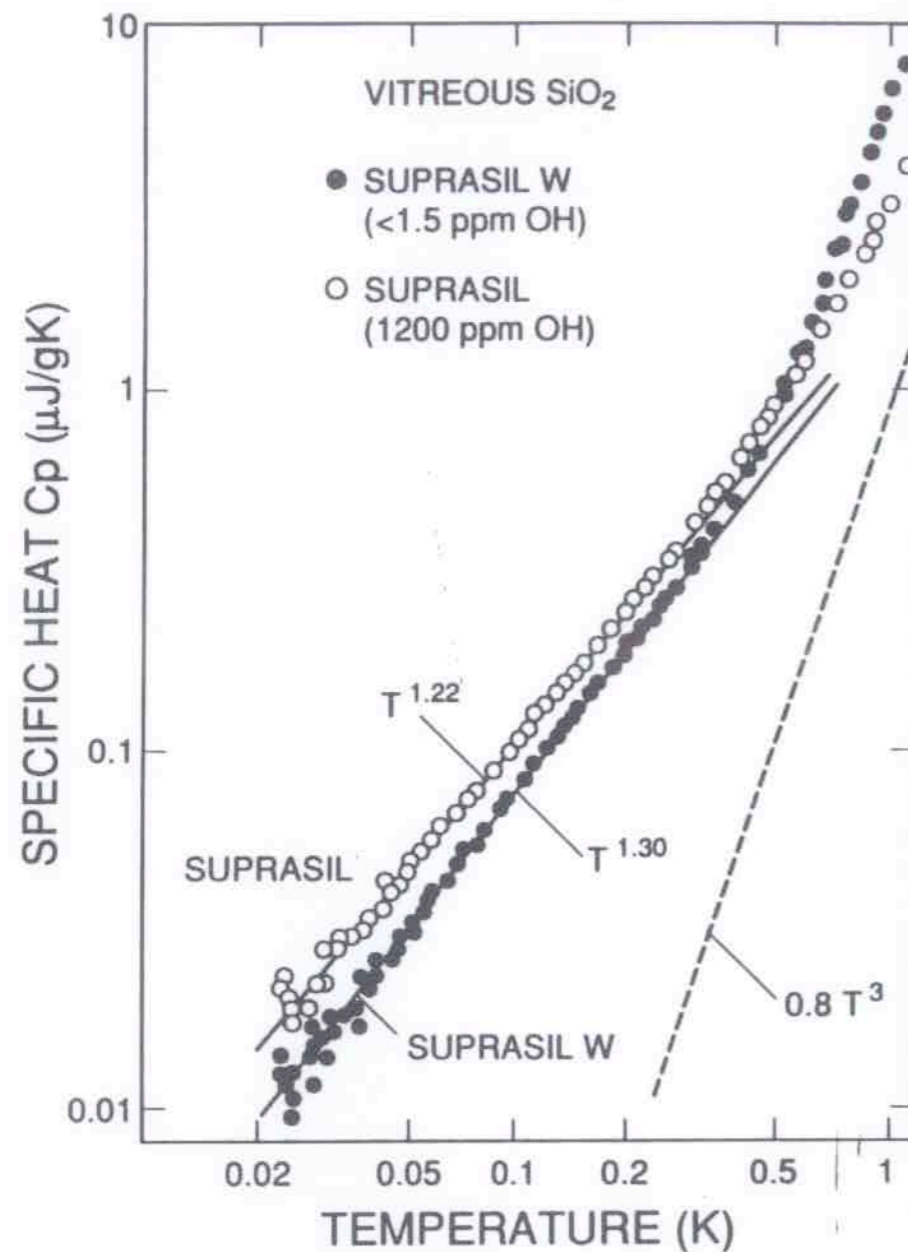


FIGURE 1 Low temperature specific heat of vitreous  $\text{SiO}_2$  from Ref. 27. Notice that the specific heat is slightly superlinear.

from Yu and Leggett  
Comments Cond. Mat. Phys.  
(1988)

# Boson peak

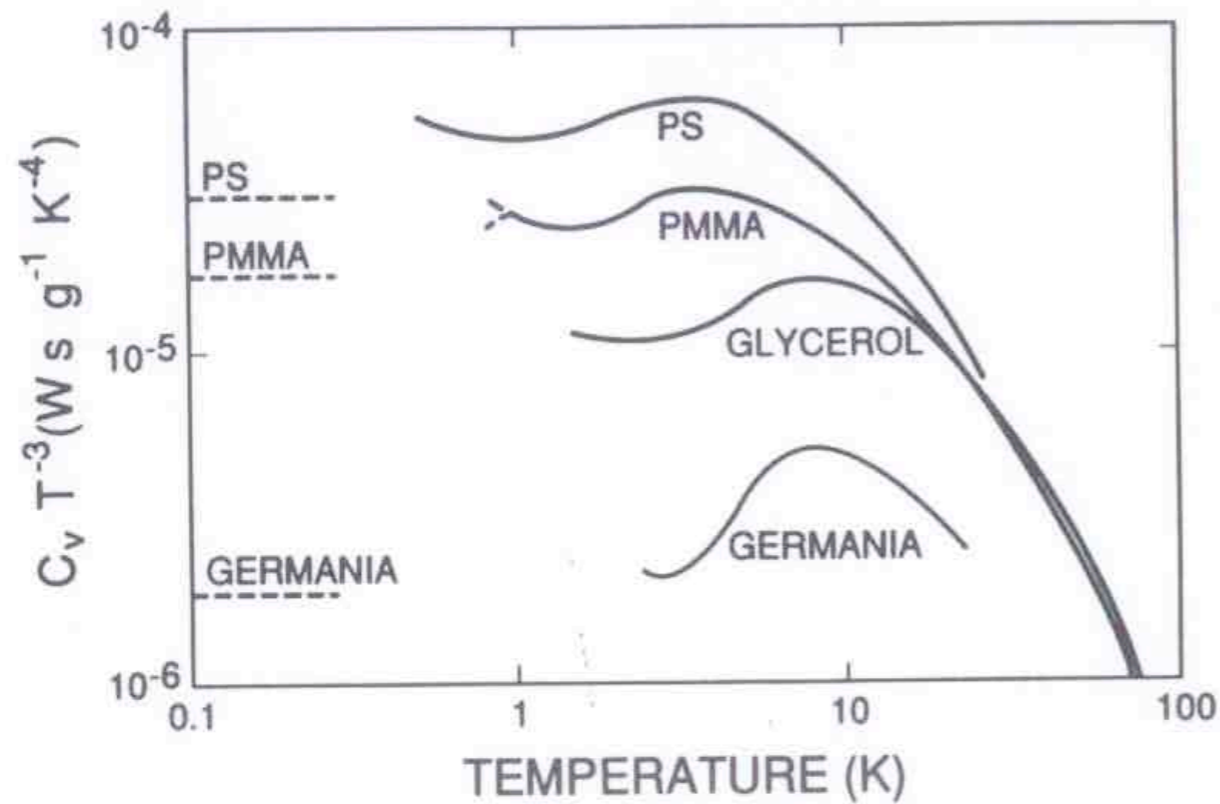


FIGURE 3  $C/T^3$  versus  $T$  from Ref. 5. Notice the bump is between 3 and 10 K.

Seen around 10 K

from Yu and Leggett  
Comments Cond. Mat. Phys.  
(1988)

# Thermal conductivity

Crystal

$T^{-1}$  Umklapp scattering

plateau

boundary scattering

$T^3$

Glass

$T^2$  term

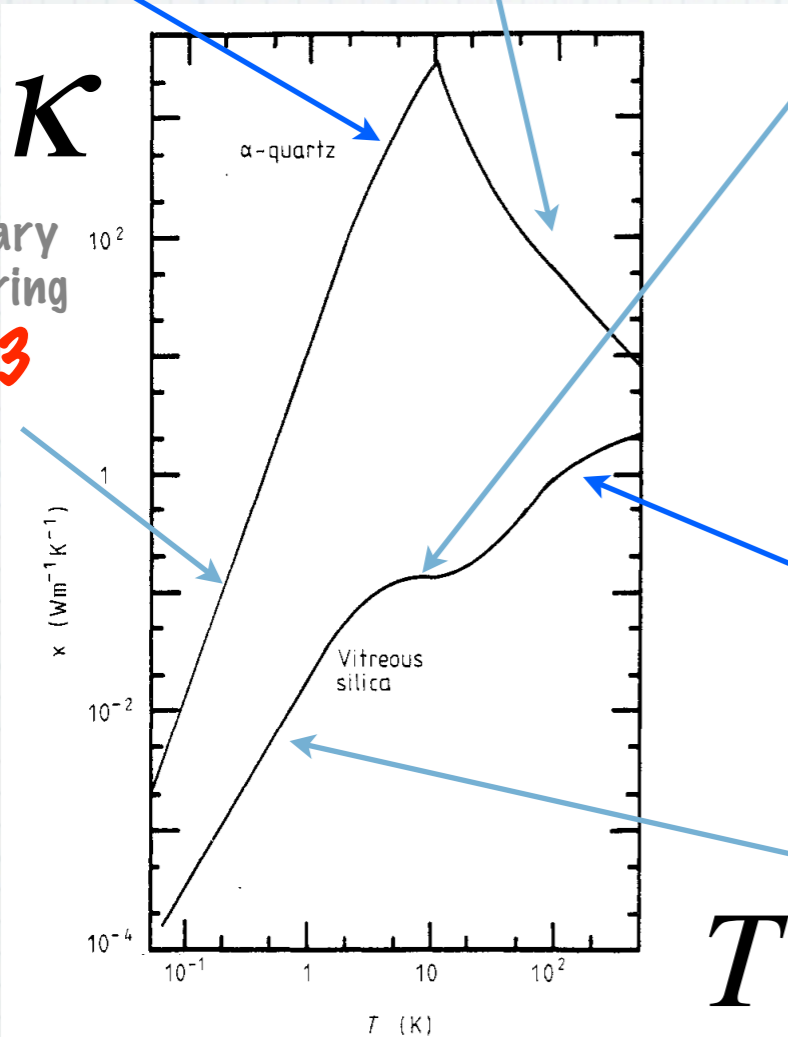
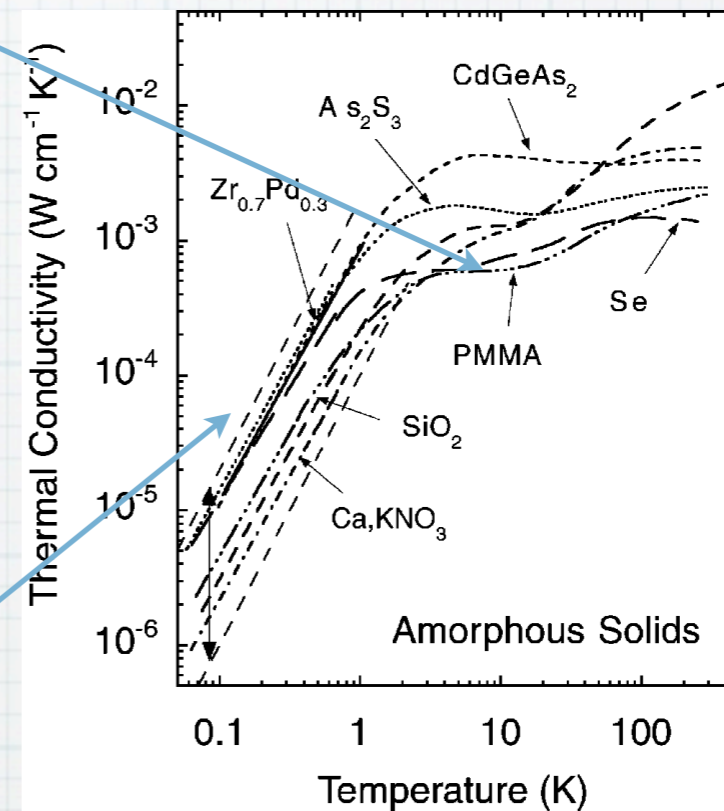


Figure 2. The thermal conductivity  $\kappa(T)$  of vitreous silica and crystalline quartz (Jones 1982, after Zeller and Pohl 1971), plotted logarithmically.



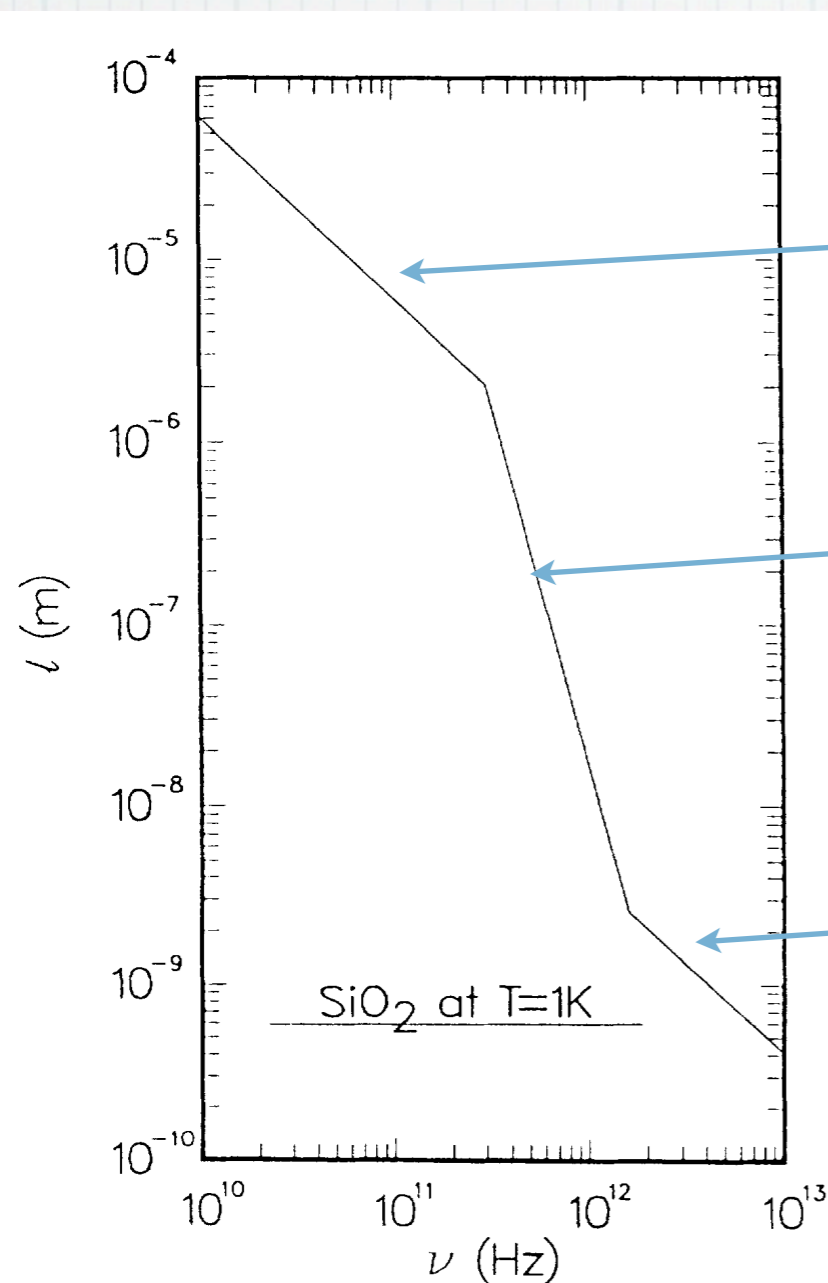
from R.O.Pohl,et.al.,RMP (2002)

from W.A.Phillips,Rep. Prog.Phys. (1987)



# Mean free path of phonons deduced from thermal conductivity

$$\kappa(T) = \frac{1}{3} \int C_{\text{ph}}(\omega) v \ell_{\text{MFP}}(\omega) d\omega$$



$$\ell_{\text{MFP}} \approx 150\lambda$$

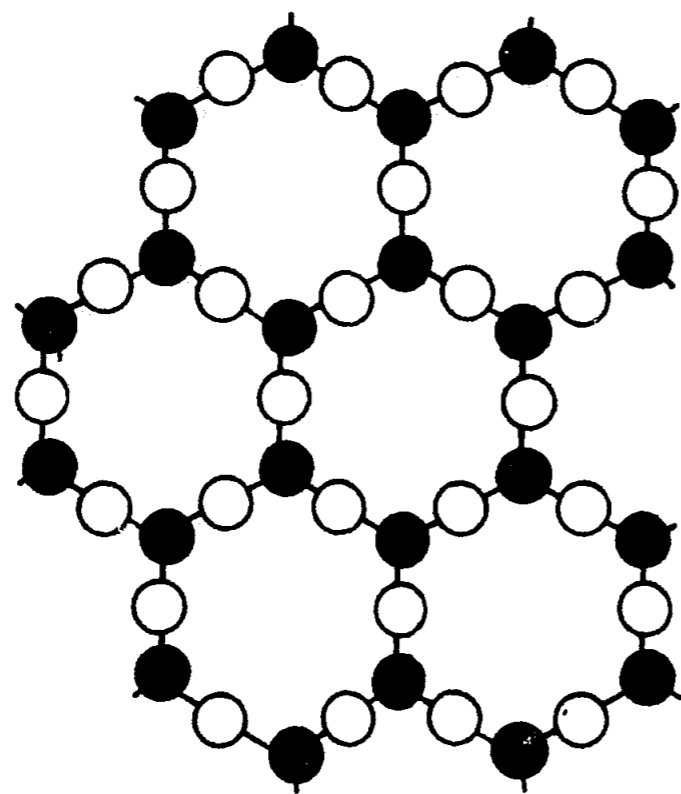
$$\ell_{\text{MFP}} \propto \lambda^4$$

$$\ell_{\text{MFP}} \propto \lambda$$

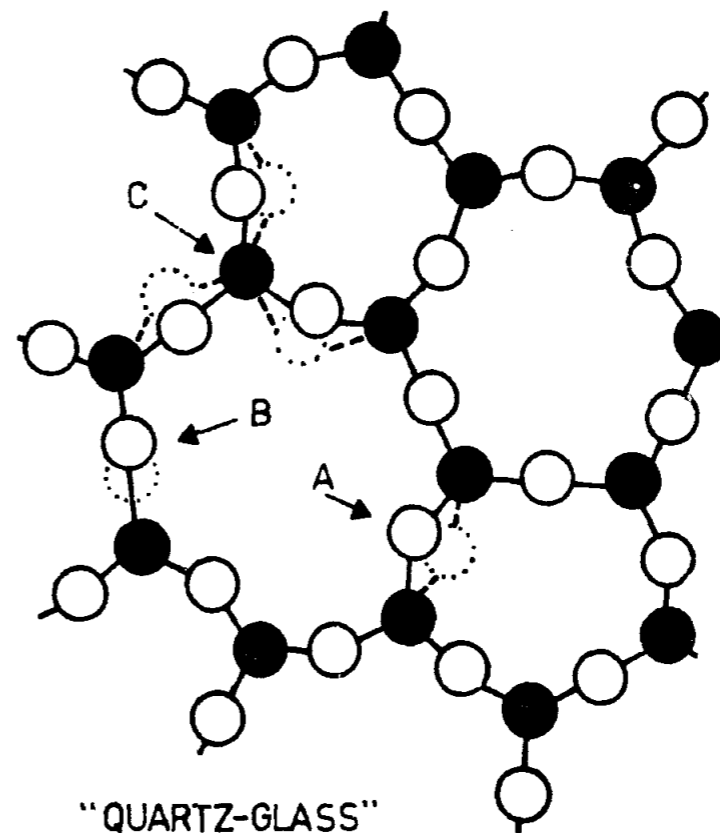
from Freeman, et al., PRB (1986)

# Explanation of these unusual properties

# Low energy excitation in glasses



"QUARTZ-CRYSTAL"

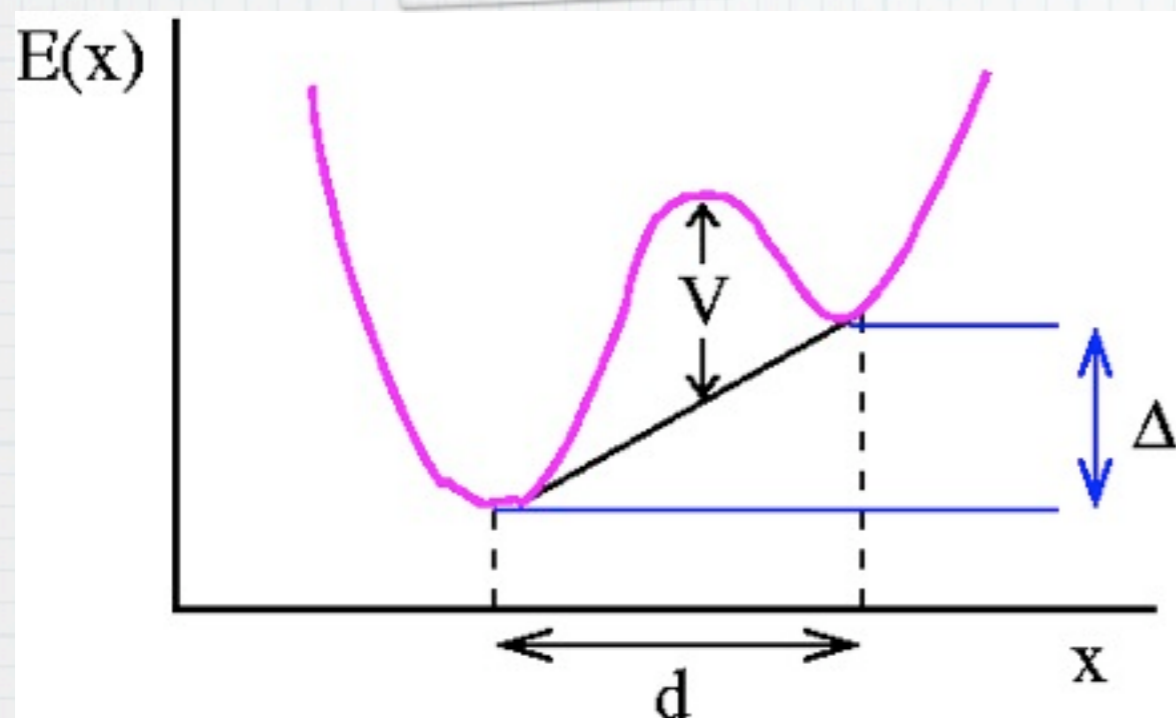


"QUARTZ-GLASS"

**Fig. 1. Schematic representation of crystalline and glassy quartz structure with three possible types of two-state defects in the glass (A, B and C) [19].**

from J.Jackle, et.al., J.Of.Non-cry. Solid. (1976)

# Two-level systems model

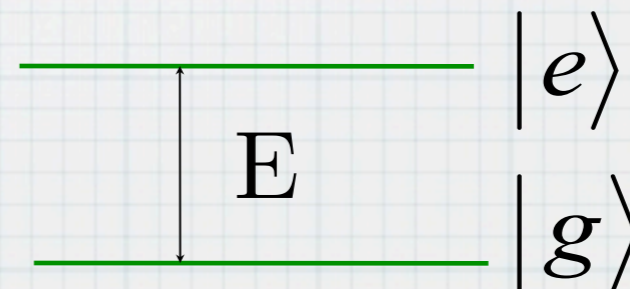


$$H = \begin{pmatrix} \Delta & \Delta_0 \\ \Delta_0 & -\Delta \end{pmatrix}$$

Asymmetry energy  $\Delta$

Tunneling energy  $\Delta_0$

$$E = \sqrt{\Delta^2 + \Delta_0^2}$$



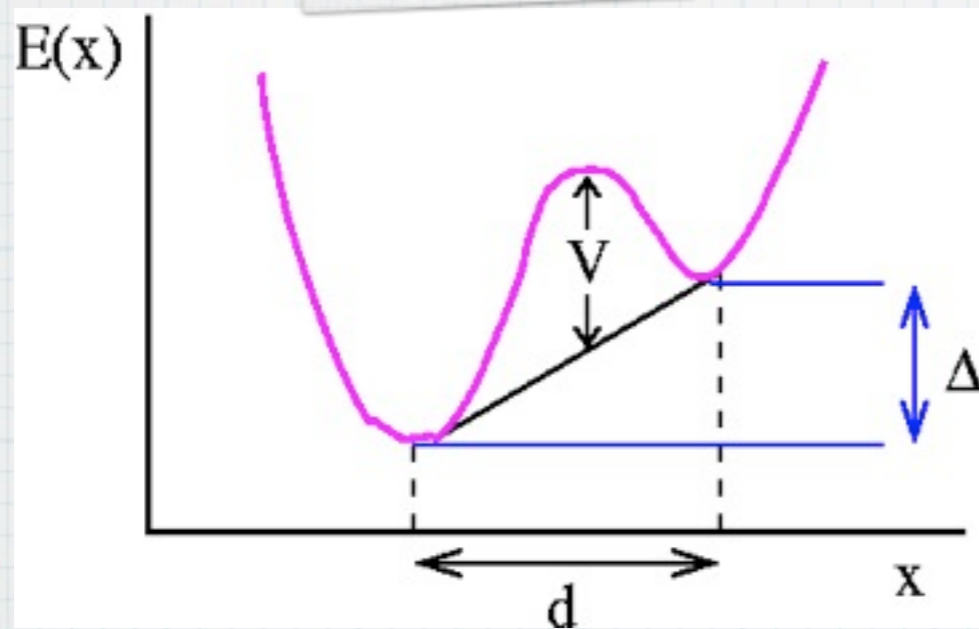
Anderson, et al., (1972),  
Phillips (1972)

# Two-Level Systems in glasses (Open question: What is the microscopic nature of TLS ?)

$\Delta$  Asymmetry energy : uniform distribution

$$\Delta_0 = \omega_0 e^{-\frac{\sqrt{2mVd}}{\hbar}}$$

Tunneling energy: barrier heights  $V$  satisfy uniform distribution (we use Gaussian distribution instead)



$\omega_0$  Zero point energy of single well

Anderson, et al., (1972),  
Phillips (1972),

# Specific heat: linear T term

Simple derivation:

occupation  
number

energy of TLS

Average  
energy

$$\bar{E}(T) = \int dE f(E) E n(E)$$

$$= n_0 \int dE \frac{1}{e^{E/k_B T} + 1} E \propto n_0 T^2$$

density of  
state of  
TLS

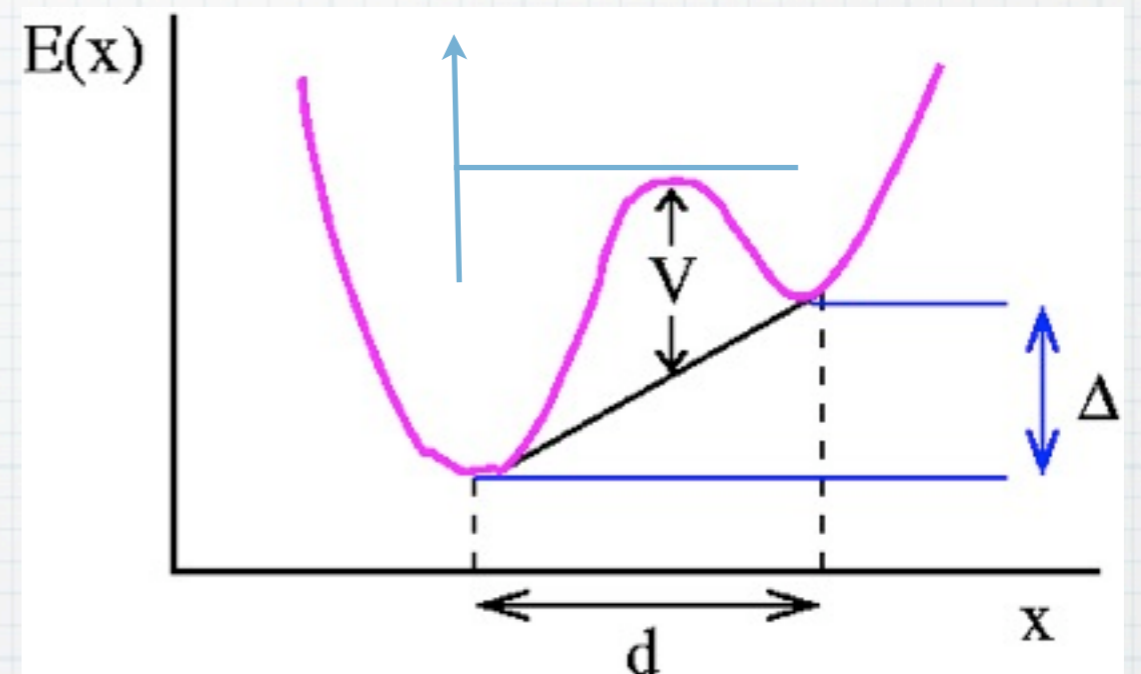
$$C(T) = \frac{\partial \bar{E}}{\partial T} \propto n_0 T$$

Anderson, et al., (1972),  
Phillips (1972)

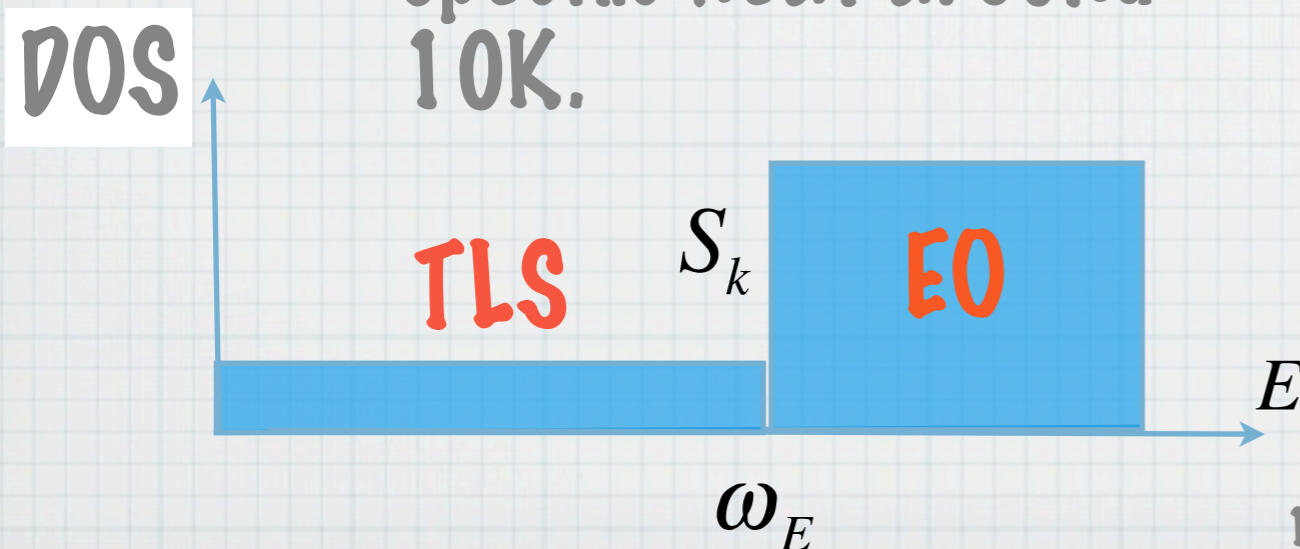
# Extend model to higher T: Einstein oscillators

\* Approximate excitations at high energy by harmonic oscillators (**Einstein oscillators = EO**).

\* EO is responsible for the peak in the specific heat around 10K.



Yu and Freeman, PRB (1987)

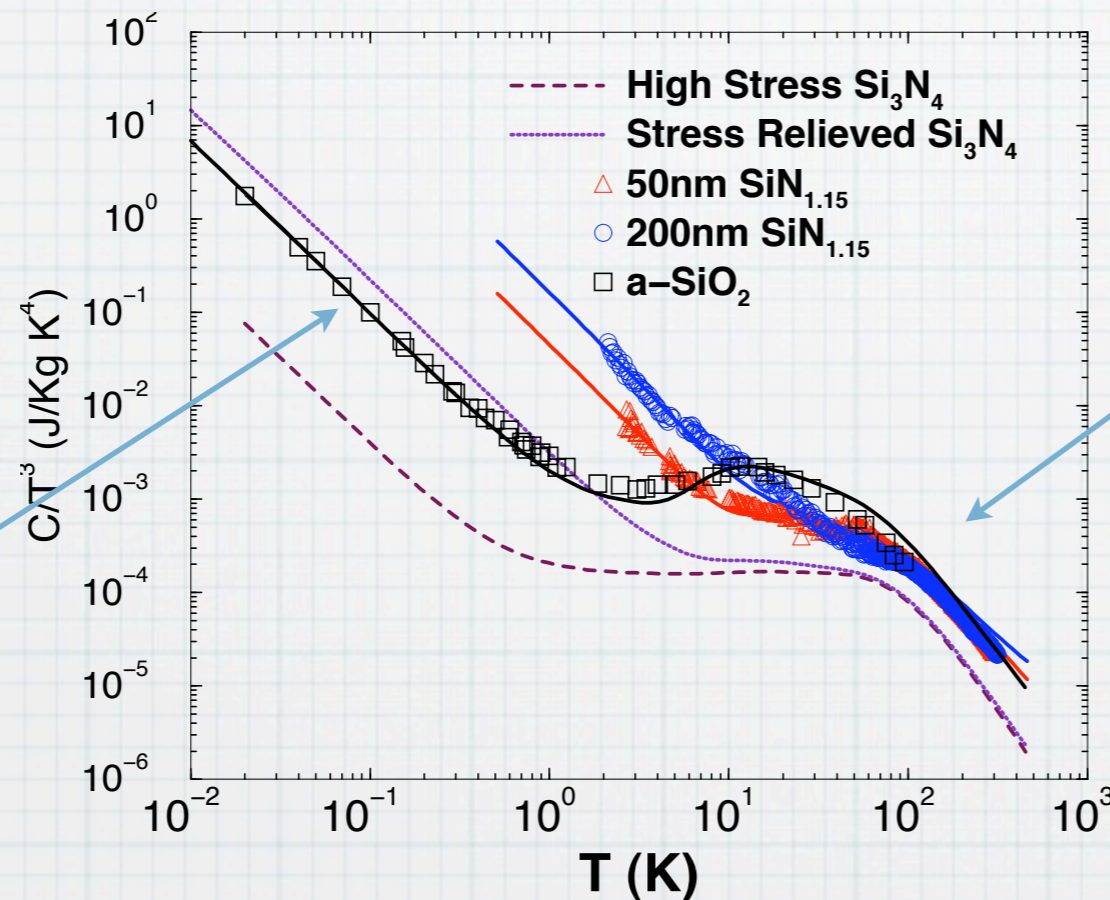


$$n(E) = n_0 [1 + S_k \Theta(E - \hbar\omega_E)]$$

# Specific heat over a broad temperature regime

$$C = C_{Debye} + C_{TLS} + C_{EO}$$

Two-Level  
Systems



Einstein  
Oscillator  
(Boson peak)

Solid and dash lines: Predicted  
 $\text{SiN}_{1.15}$ : from Southworth, et al., PRL (2009)  
a-SiO<sub>2</sub>: from Yu and Freeman, RPB (1987)



# Thermal conductivity

Heat is transported by phonons in glasses (Zaitlin and Anderson, 1975)

$$\kappa(T) = \frac{1}{3} \int C_{\text{ph}}(\omega) v \ell_{\text{MFP}}(\omega) d\omega$$

How much energy  
a phonon can carry

How fast  
a phonon goes

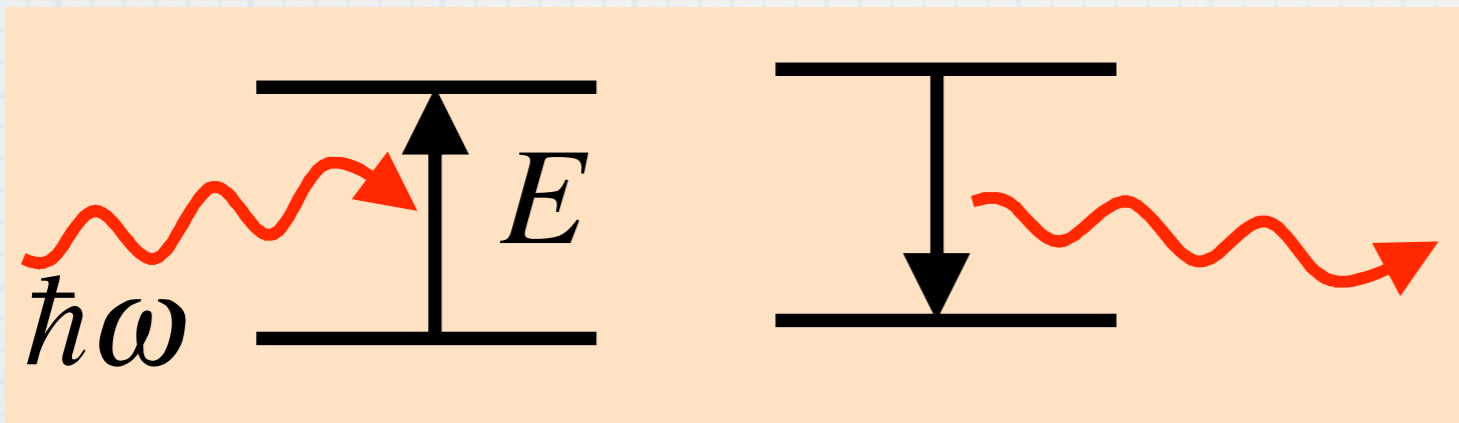
How far  
a phonon can go  
before it hits something

# Resonant scattering of TLS

Phonons (photons) are absorbed and emitted when a TLS is excited and de-excited

$$\ell_{MFP, \text{Resonance}}^{-1} = \alpha \omega \tanh\left(\frac{\hbar \omega}{2k_B T}\right) \sim \omega \text{ for } \hbar \omega \gtrsim k_B T$$

$$\alpha = \frac{\pi \bar{P} \gamma^2}{\rho v^3}$$



$$\hbar \omega = E$$

$\bar{P}$  spectral density  
(density of TLS)

$\gamma$  deformation potential  
(coupling of TLS and phonons)

# Thermal conductivity goes as $T^2$ at low temperatures

$$\kappa(T) = \frac{1}{3} \int C_{\text{ph}}(\omega) v \ell_{\text{MFP}}(\omega) d\omega$$

Debye theory

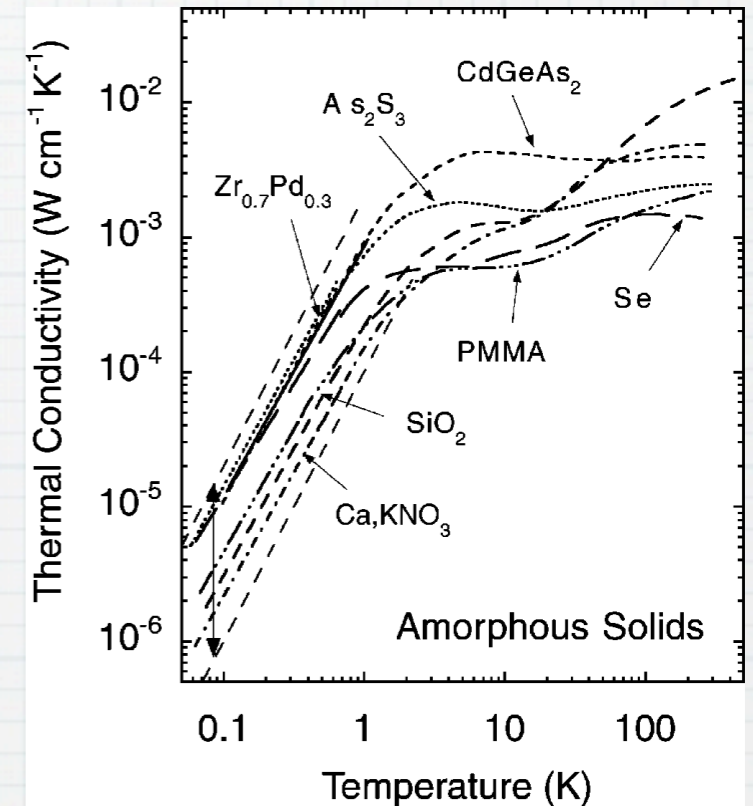
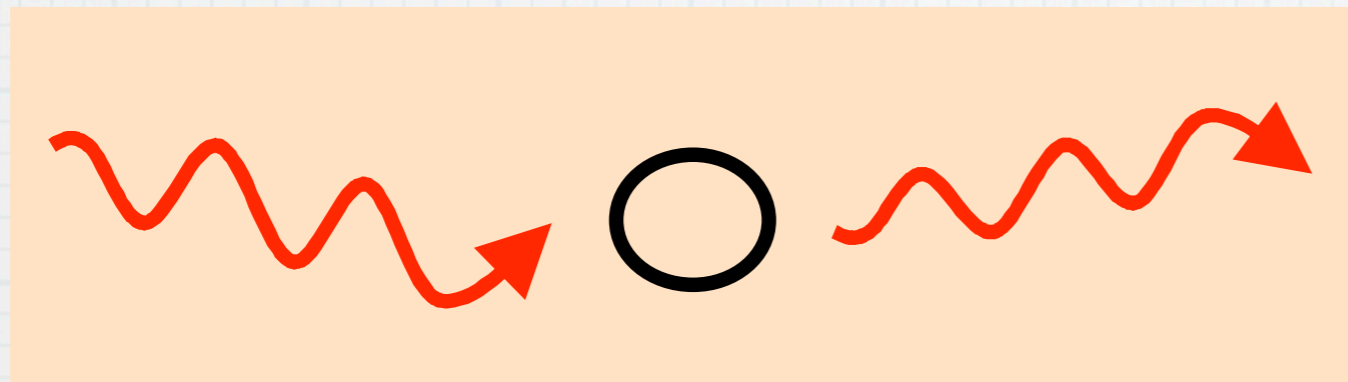
$$T^3$$

$$\ell_{\text{MFP}} \propto \frac{1}{\omega} \sim \frac{1}{T}$$

$$\kappa(T) \propto T^2$$

# Plateau in thermal conductivity

Plateau dominated by Rayleigh scattering of phonons



Phonons (photons) are scattered by atoms or small size defects

$$\ell_{MFP, \text{Rayleigh}}^{-1} = B\omega^4$$

# Four mechanisms contribute to phonon scattering

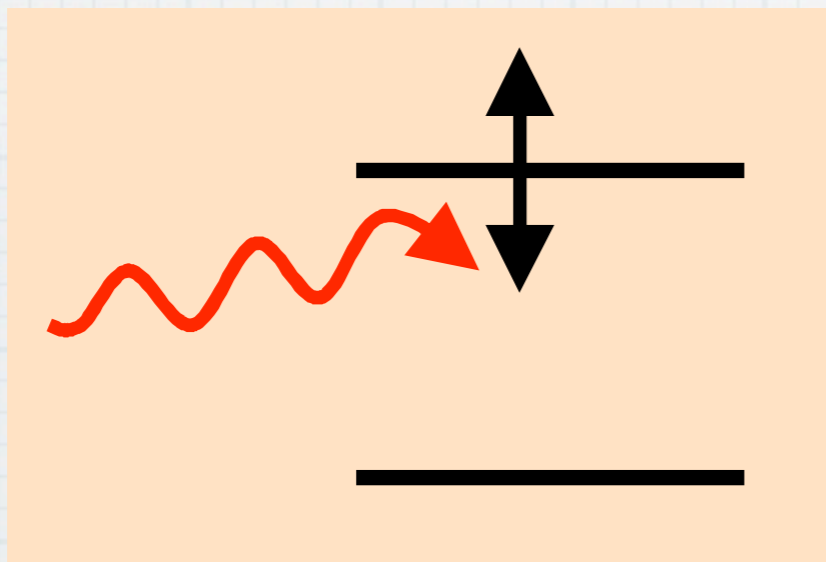
- \* Resonant scattering of phonons from TLS
- \* **TLS relaxation**
- \* Rayleigh scattering
- \* **Scattering from Einstein oscillators**

$$\ell_{MFP}^{-1} = \left\{ \begin{array}{l} \ell_{MFP,Resonant}^{-1} + \ell_{MFP,Relaxation}^{-1} + \ell_{MFP,Rayleigh}^{-1} \quad \omega < \omega_E \\ \ell_{MFP,Resonant}^{-1} + \ell_{MFP,Relaxation}^{-1} + \ell_{MFP,Einstein}^{-1} \quad \omega > \omega_E \end{array} \right\}$$

**Combining two models: Yu-Freeman, PRB (1987) & Hunklinger, PRB (1992)**

# Phonon scattering due to TLS relaxation (dominates at low frequencies)

Phonons (photons) modulate TLS energy splitting. TLS population redistributes to achieve new equilibrium.



$$P(\Delta, V) = \frac{\bar{P}}{E_0} e^{-\frac{(V-V_0)^2}{2\sigma_0^2}}$$

$$\ell_{MFP, \text{Relaxation}}^{-1} = \frac{\alpha\omega}{\pi} \int dV \int_0^{2V} d\Delta P(\Delta, V) \sec h^2 \left( \frac{\hbar\omega}{2k_B T} \right) \left( \frac{\Delta}{E} \right)^2 \frac{\omega\tau}{1 + (\omega\tau)^2}$$

# Two processes of TLS relaxation

## Relaxation time

$$\tau^{-1} = \tau_{\text{Tunneling}}^{-1} + \tau_{\text{Thermal Activation}}^{-1}$$

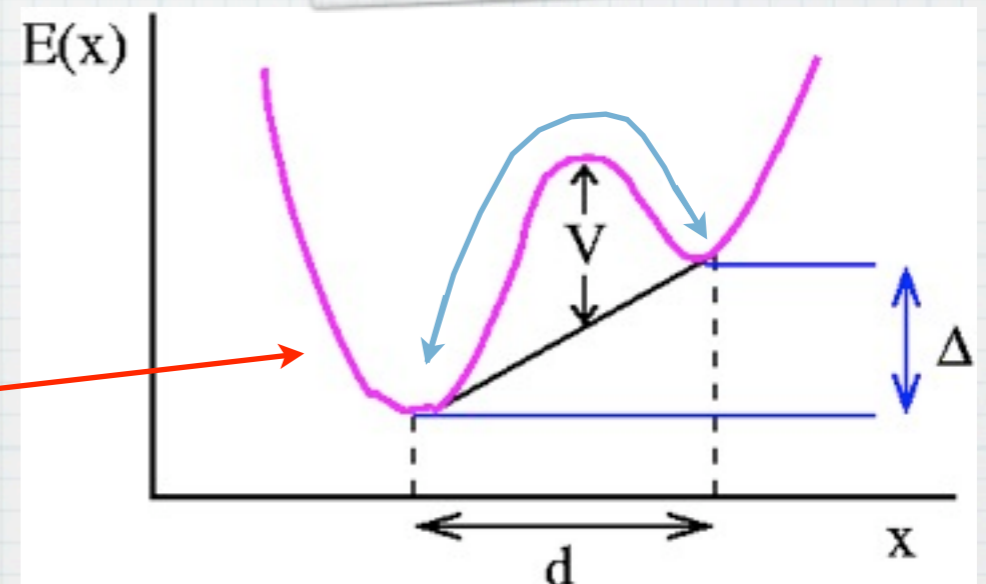
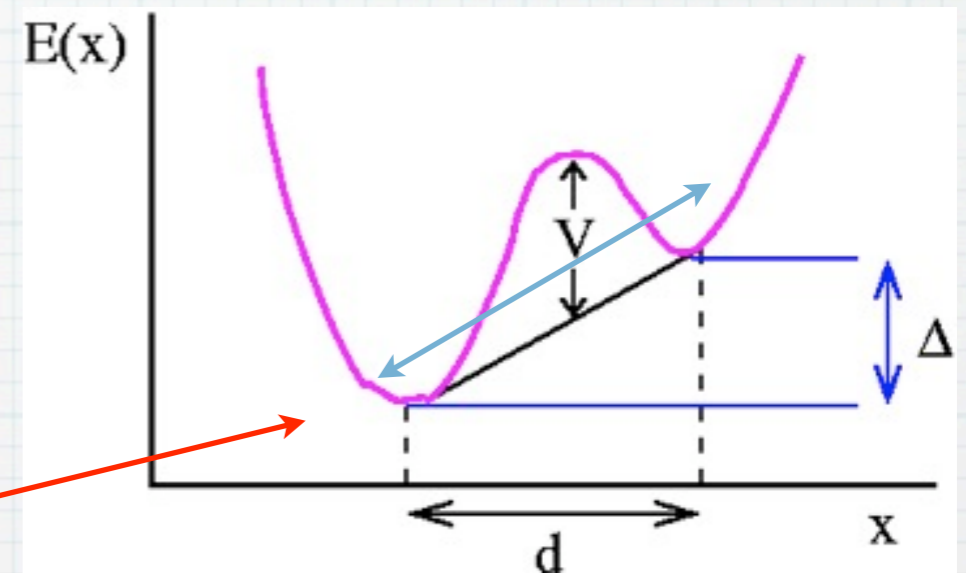
## Tunneling

$$\Delta_0 = \omega_0 e^{-\frac{\sqrt{2mVd}}{\hbar}}$$

$$\tau_{\text{Tunneling}}^{-1} = A\Delta_0^2 E \coth\left(\frac{\hbar\omega}{2k_B T}\right)$$

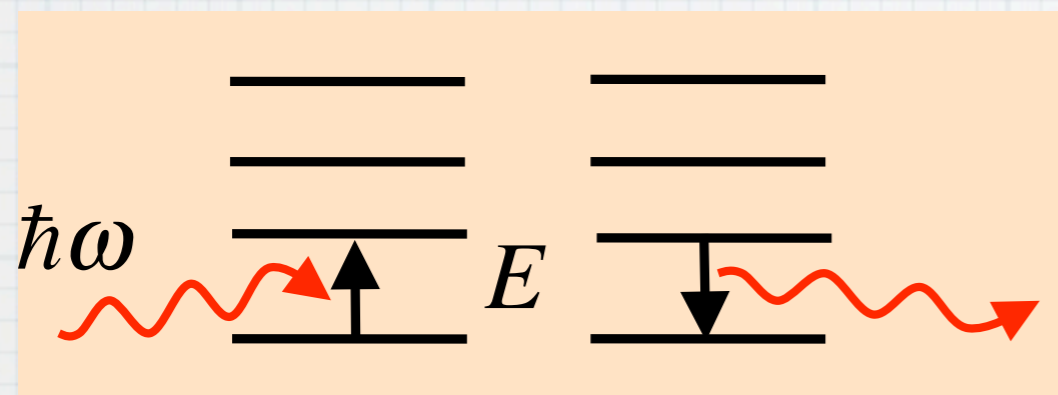
## Thermal activation

$$\tau_{\text{Thermal Activation}}^{-1} = \tau_0^{-1} \cosh\left(\frac{\Delta}{2k_B T}\right) e^{-V/2k_B T}$$



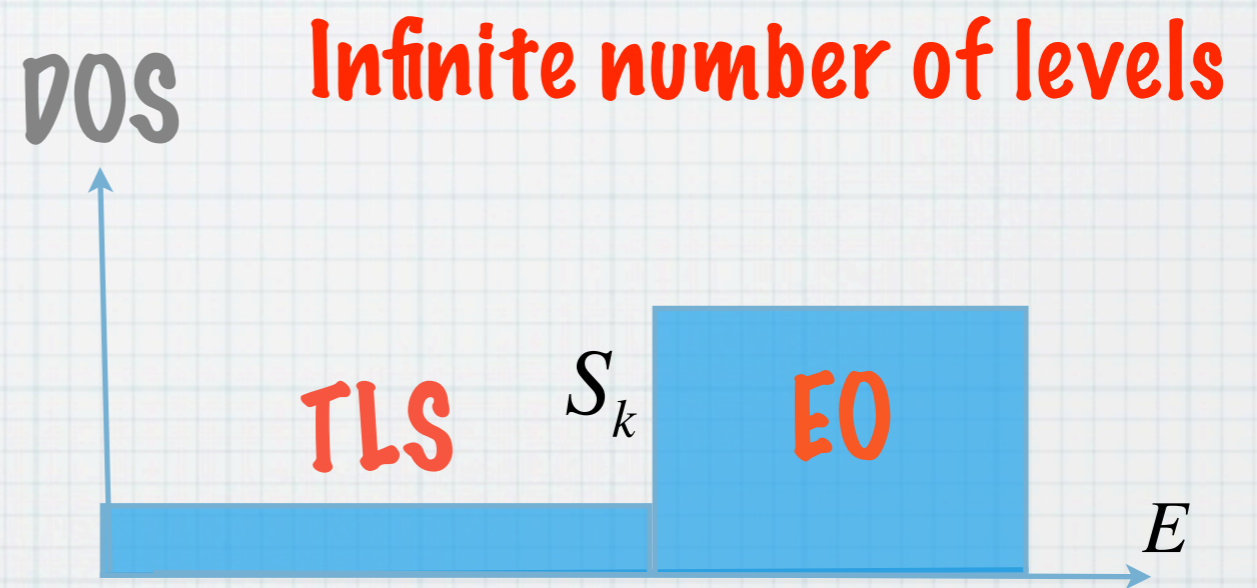
# Phonon scattering from Einstein oscillators

Phonons (photons) are absorbed and emitted when a harmonic oscillator is excited and de-excited



$$\hbar\omega = E$$

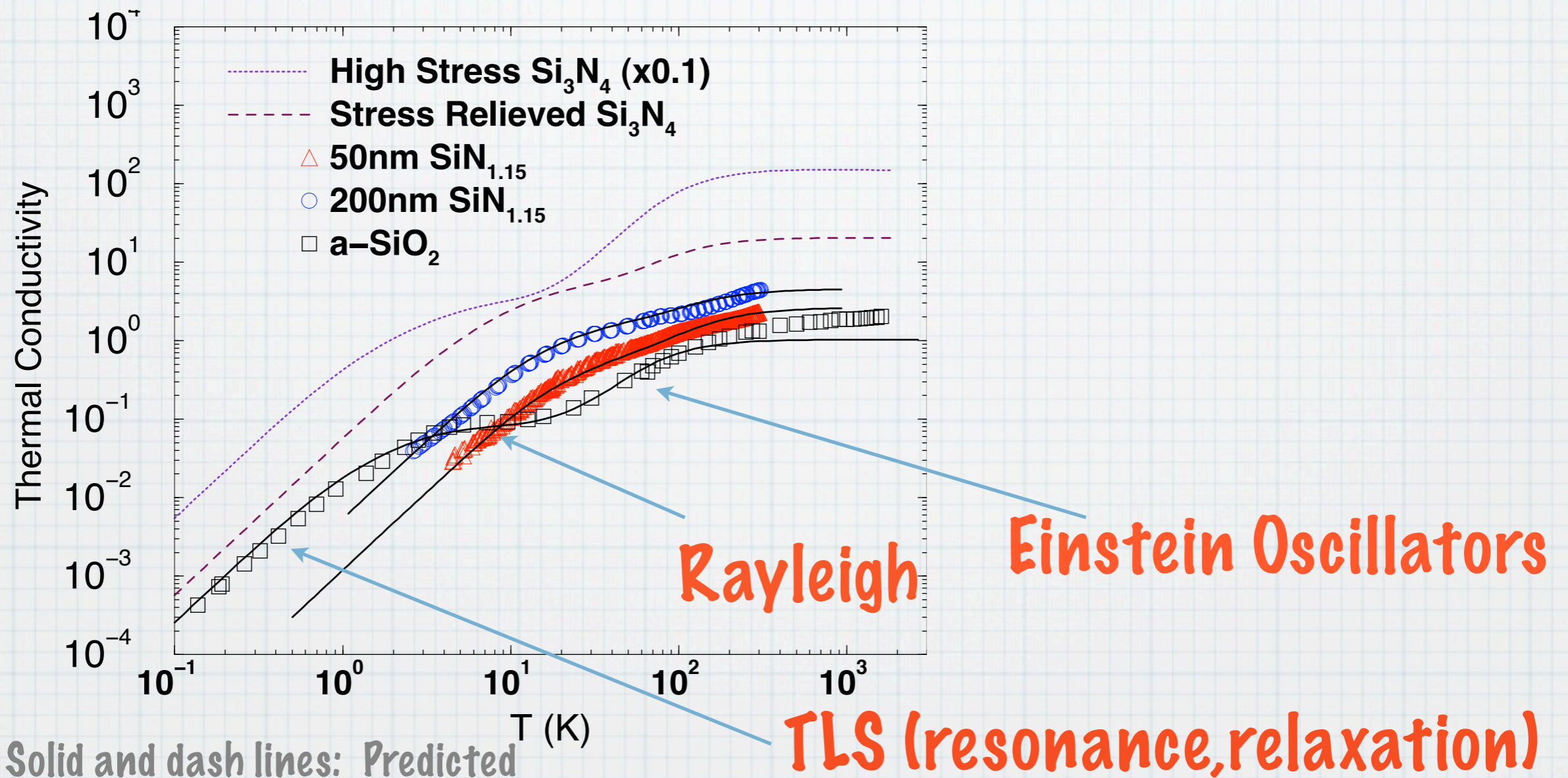
$$\ell_{MFP, Einstein}^{-1} = \frac{2\alpha S_k}{\pi} \omega$$



$$n(E) = n_0 [1 + S_k \Theta(E - \hbar\omega_E)]$$



# Thermal conductivity

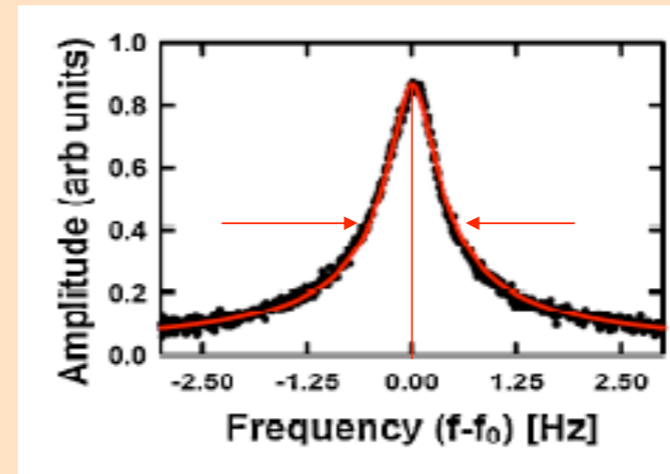
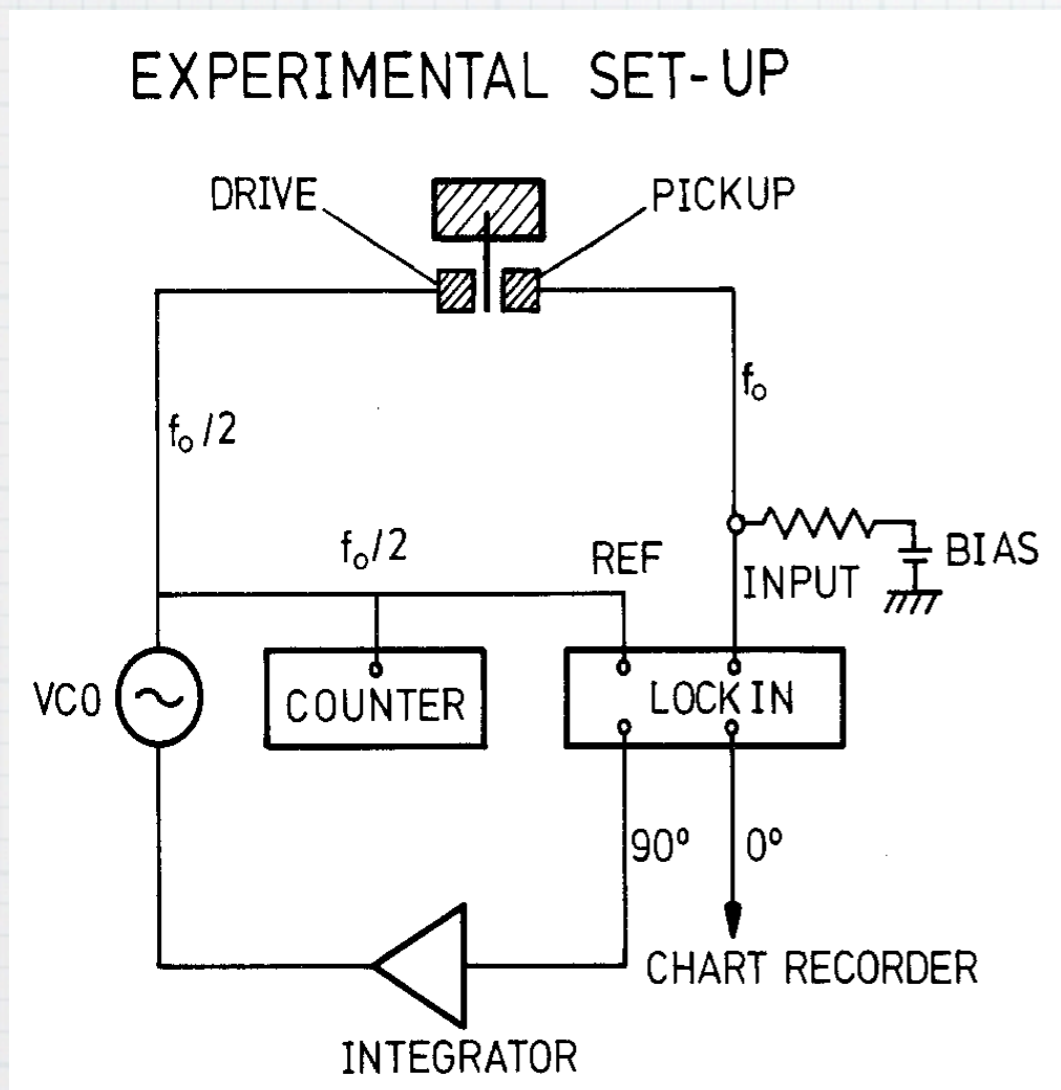


Solid and dash lines: Predicted  
 $\text{SiN}_{1.15}$ : from Southworth, et al., PRL (2009)  
a- $\text{SiO}_2$ : from Yu and Freeman, RPB (1987)

# Introduction to acoustic dissipation in glasses

# How to measure the dissipation in glasses

# Measuring acoustic dissipation in glasses



$\Delta f$

$f_0$

Quality factor  
(internal friction)  $Q^{-1} = \frac{f_0}{\Delta f}$

Raychaudhuri, et al.  
Z.Phys.B (1984)

# Universal dissipation in glasses

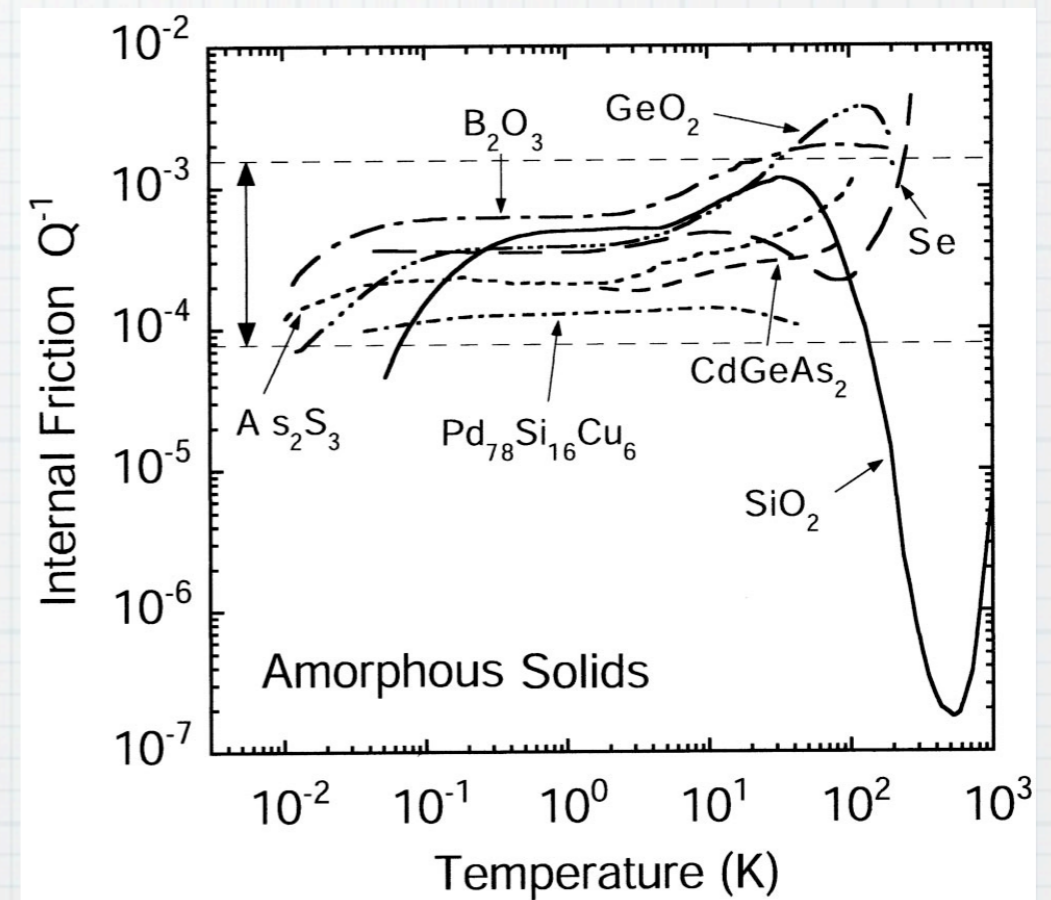
For various glasses such as  $\text{SiO}_2$ ,  $\text{B}_2\text{O}_3$ ,...at  $0.1\text{K} < T < 10\text{K}$

$$Q^{-1} \sim 10^{-4} - 10^{-3}$$

Due to two-level-systems (TLS) at low temperatures

Anderson, et al., (1972), Phillips (1972), Jackle (1972)

Zeller, et al., PRB (1971)

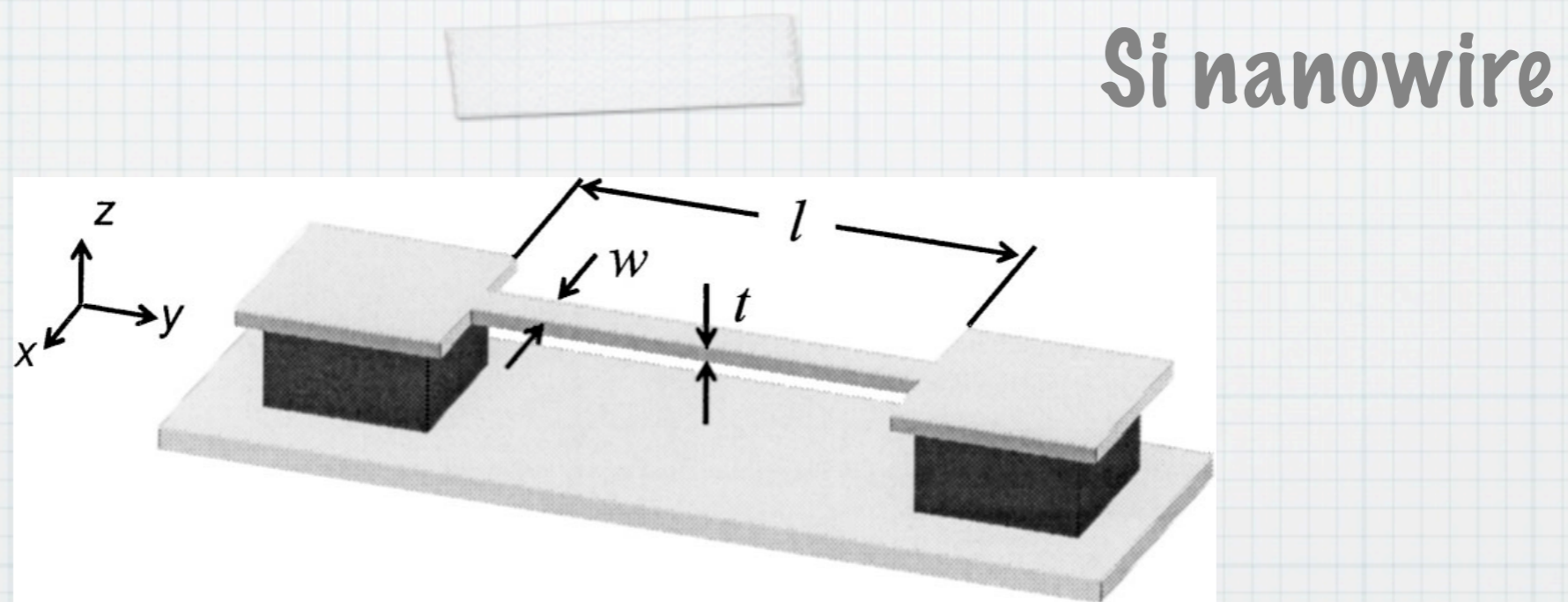


R.O.Pohl, et al., RMP (2002)

**Why do we want to reduce  
the dissipation in glasses?**

# Motivation: high $Q$ (low dissipation) is important!

- \* Example 1: Resonant mass sensor (  $Q$  will determine the minimum mass detectable)

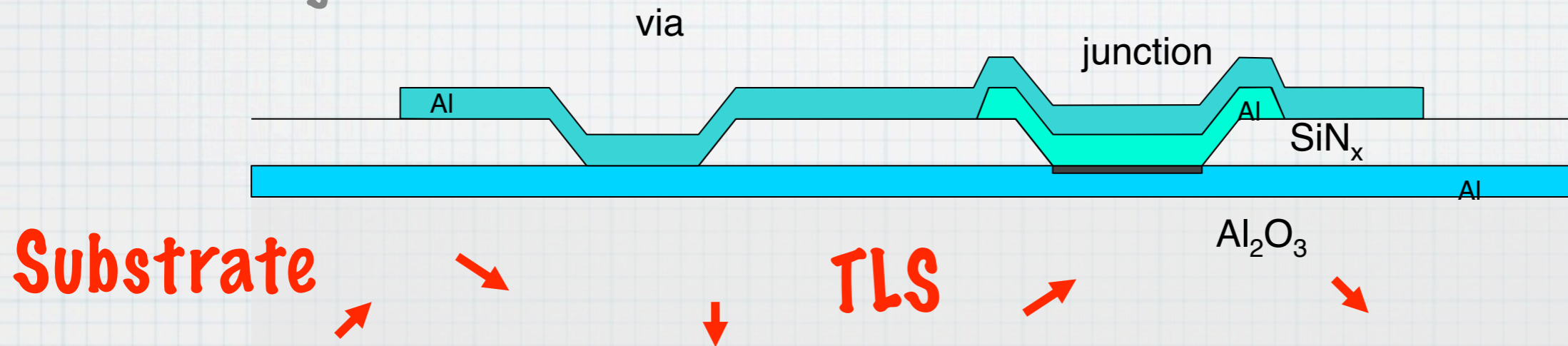


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from Ekinici, et al., JAP (2004)

# Motivation: high Q (low dissipation) is important!

- \* Example 2: SQUIDs are used as qubits; need to reduce the noise.
- \* Charge noise is proportional to the dielectric loss tangent of substrate.



Martinis, et al., PRL (2005)

In glasses, at low temperature and low frequency, acoustic dissipation (phonons) and dielectric loss (photons) are all due to TLS.

S. Hunklinger, PLTP (1984)

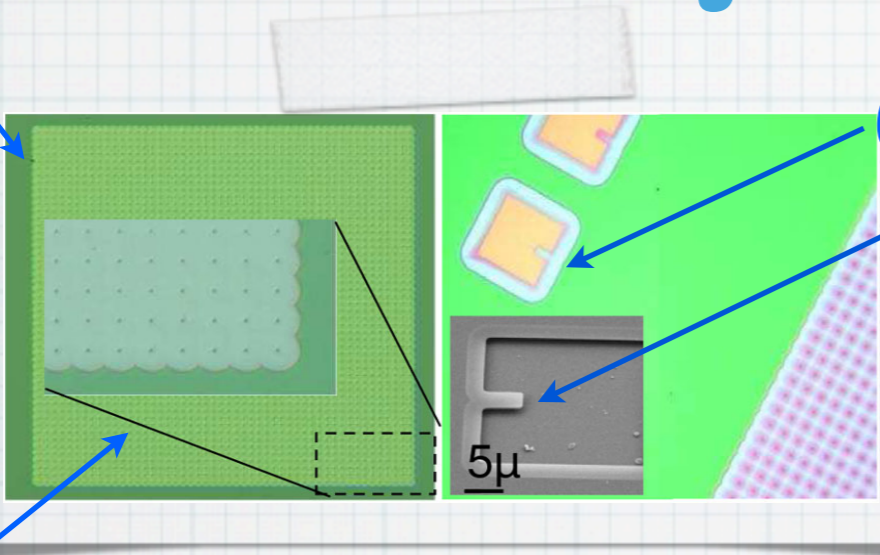


Since dissipation is  
ubiquitous in glasses,  
can we reduce it?

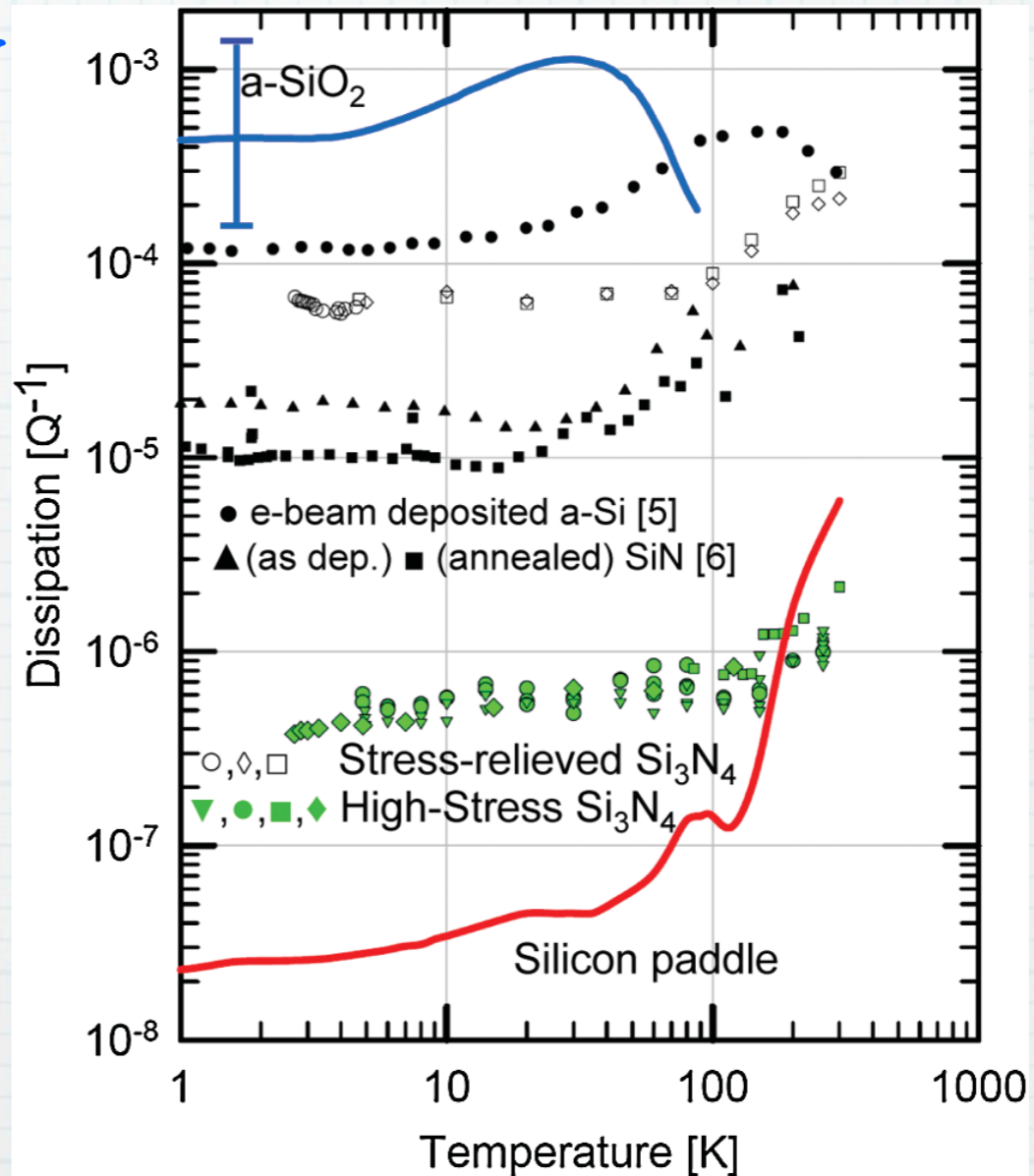
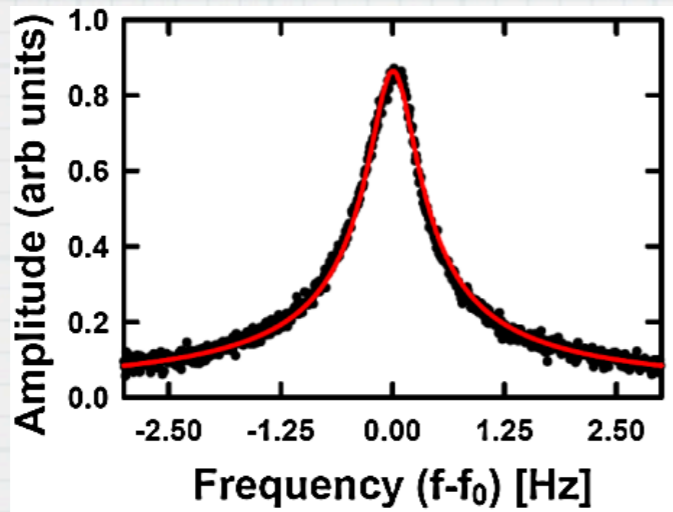
# Yes! Anomalously low dissipation in $\text{Si}_3\text{N}_4$

wafer

Cantilever



drumhead



D.R. Southworth, et.al., PRL  
(2009)

# Two questions to answer

- \* Why does high stress reduce dissipation of  $\text{Si}_3\text{N}_4$  so dramatically ?
- \* Why does stress-relieved  $\text{Si}_3\text{N}_4$  have an order of magnitude lower in dissipation than  $\text{SiO}_2$  ?

**Why does high stress reduce the dissipation in glasses ?**

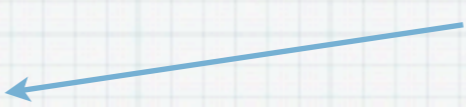
**Answer:**

Relaxation via tunneling and thermal activation is exponentially sensitive to  $V$ . High stress increases the barrier heights  $V$ , effectively reducing the number of defects that produce dissipation.

# Theory of dissipation in glasses

$$Q^{-1} = \frac{\lambda}{\ell_{\text{MFP}}}$$

phonon wave length



Dissipation and thermal conductivity are all related to the mean free path of phonons (photons)

# Four mechanisms contribute to the dissipation

$$0.1K < T < 10K$$

$$\omega \sim 1 \text{ MHz}$$

- \* **Resonant scattering of phonons from TLS**  $Q_{\text{Resonance}}^{-1} \sim 10^{-7}$
- \* **TLS relaxation**  $Q_{\text{Relaxation}}^{-1} \sim 10^{-3}$  ✓
- \* **Rayleigh scattering**  $Q_{\text{Rayleigh}}^{-1} \sim 10^{-18}$
- \* **Scattering from Einstein oscillators** **Only involved at high T**

**Therefore, relaxation dominates**

# Dissipation due to TLS relaxation

$$Q_{\text{Relaxation}}^{-1} = \frac{2Q_0^{-1}}{\pi} \int dV \int_0^{2V} d\Delta P(\Delta, V) \operatorname{sech}^2 \left( \frac{\hbar\omega}{2k_B T} \right) \left( \frac{\Delta}{E} \right)^2 \frac{\omega\tau}{1 + (\omega\tau)^2}$$

## Relaxation time

$$\tau^{-1} = \tau_{\text{Tunneling}}^{-1} + \tau_{\text{Thermal Activation}}^{-1}$$

## Tunneling

$$\tau_{\text{Tunneling}}^{-1} = A\Delta_0^2 E \coth \left( \frac{\hbar\omega}{2k_B T} \right) \quad \Delta_0 = \omega_0 e^{-\frac{\sqrt{2mVd}}{\hbar}}$$

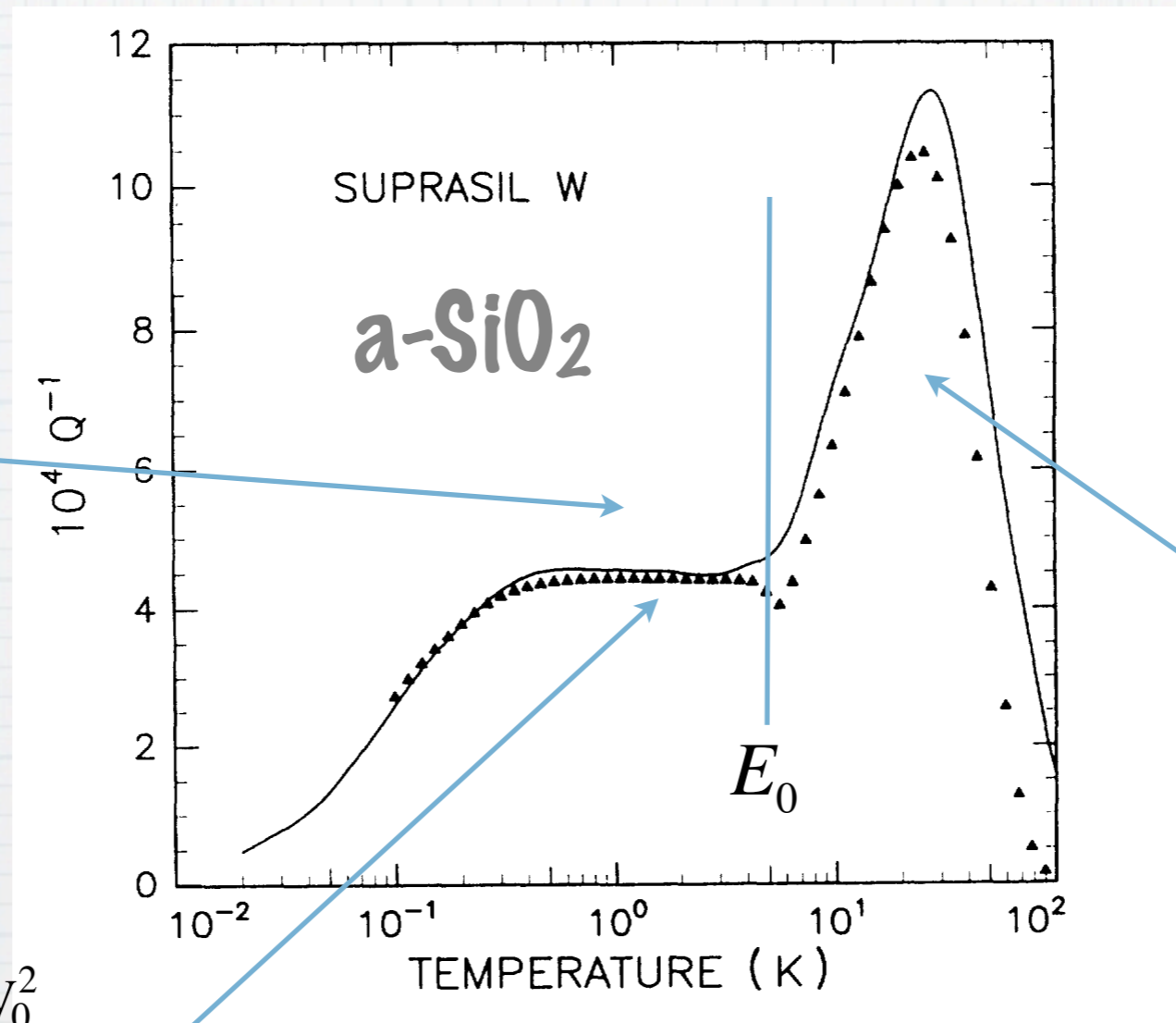
## Gaussian distribution of barrier heights $V$

## Thermal activation

$$\tau_{\text{Thermal Activation}}^{-1} = \tau_0^{-1} \cosh \left( \frac{\Delta}{2k_B T} \right) e^{-V/2k_B T}$$

$$P(\Delta, V) = \frac{\bar{P}}{E_0} e^{-\frac{(V-V_0)^2}{2\sigma_0^2}}$$

# Dissipation at low temperature



Tunneling

Universal

Thermal activation

$$Q_0^{-1} \approx \frac{\pi \bar{P} \gamma^2}{2\rho v^2} e^{-\frac{V_0^2}{2\sigma_0^2}}$$

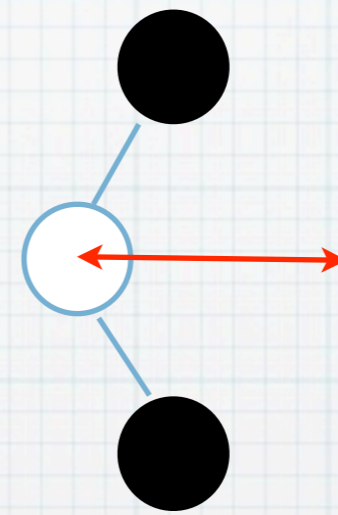
S. Hunklinger, PRB (1992)



# Why low stress $\text{Si}_3\text{N}_4$ has low dissipation compared with $\text{SiO}_2$ ?

3- or 4-fold coordinated materials will have extra constraints, producing non-relieved strain energy, thus increasing the barrier heights.  $V_0$  is nonzero compared to a- $\text{SiO}_2$

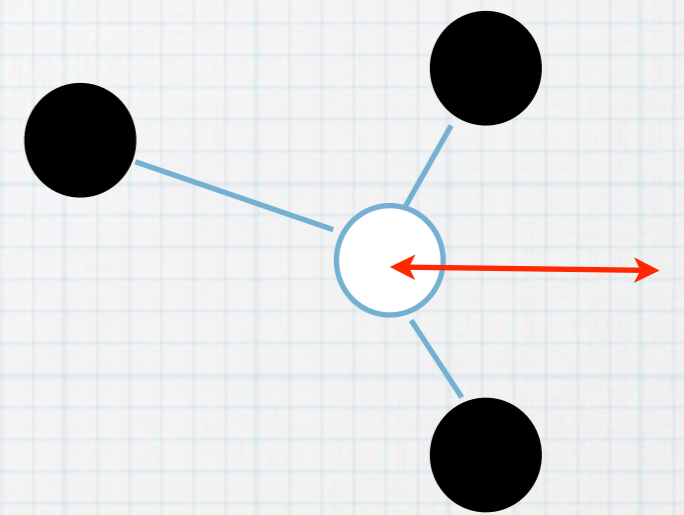
$$P(\Delta, V) = \frac{\bar{P}}{E_0} e^{-\frac{(V-V_0)^2}{2\sigma_0^2}}$$



a- $\text{SiO}_2$

$$V_0 = 0K$$

$$\sigma_0 = 445K$$



$\text{Si}_3\text{N}_4$

$$V_0 = 13500K$$

$$\sigma_0 = 9000K$$

# Why high stress can reduce dissipation in glasses ?

High stress increases the strain energy, thus increasing the barrier heights.  $V_0$  is increased compared with low stress

$\text{Si}_3\text{N}_4$

# Dissipation of Si<sub>3</sub>N<sub>4</sub>

Si<sub>3</sub>N<sub>4</sub>: Queen, et al., RSI (2009)

a-SiO<sub>2</sub>: from Yu and Freeman, RPB (1987)

$$V_0 = 0K$$

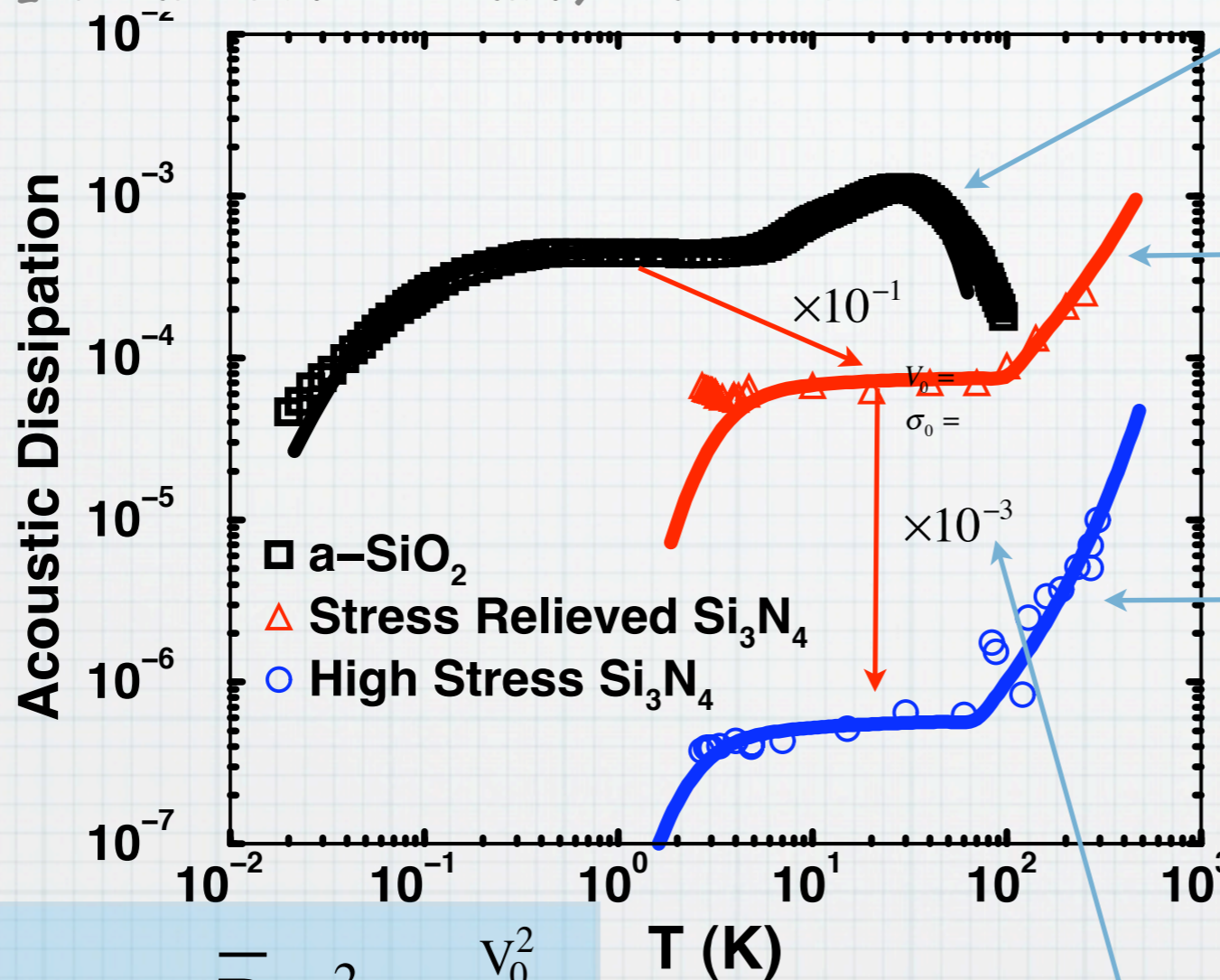
$$\sigma_0 = 445K$$

$$V_0 = 13500K$$

$$\sigma_0 = 9000K$$

$$V_0 = 25300K$$

$$\sigma_0 = 7500K$$



$$P(\Delta, V) = \frac{\bar{P}}{E_0} e^{-\frac{(V-V_0)^2}{2\sigma_0^2}}$$

$$Q_0^{-1} \approx \frac{\pi \bar{P} \gamma^2}{2\rho v^2} e^{-\frac{V_0^2}{2\sigma_0^2}}$$

high stress

# Conclusion

- \* Universal properties of glasses, such as dissipation, specific heat, and thermal conductivity can be well described by a **two level system and Einstein oscillator model**.
- \* Glasses made of **3- or 4-fold coordinated materials** and glasses in the presence of **high stress** can have very low dissipation.
- \* High stress increases barrier heights of defects, effectively reducing the number of defects producing dissipation.