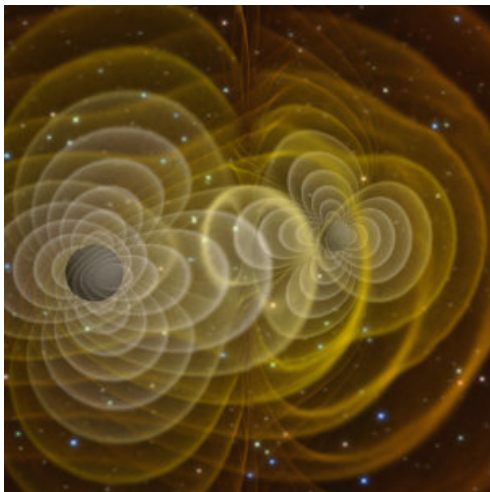


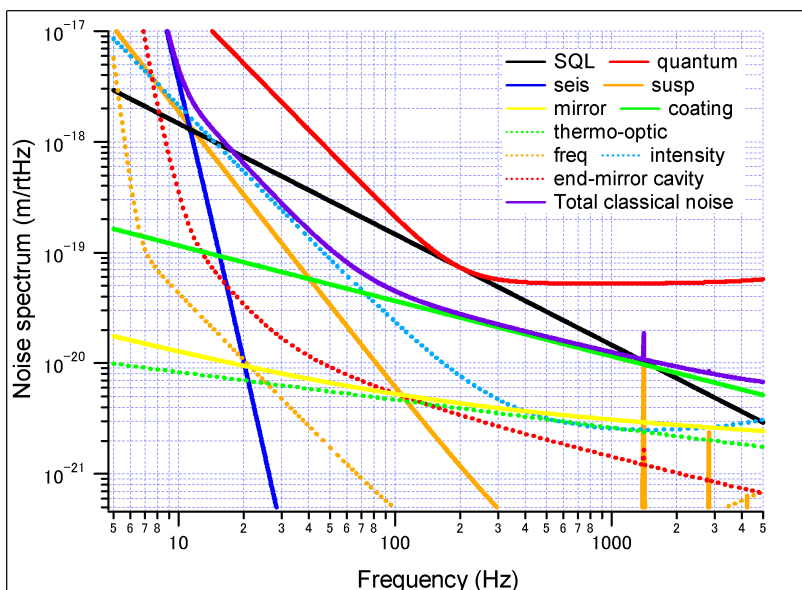
# Modeling Internal Friction in Amorphous Oxides Using Two-Level Systems

Chris Billman

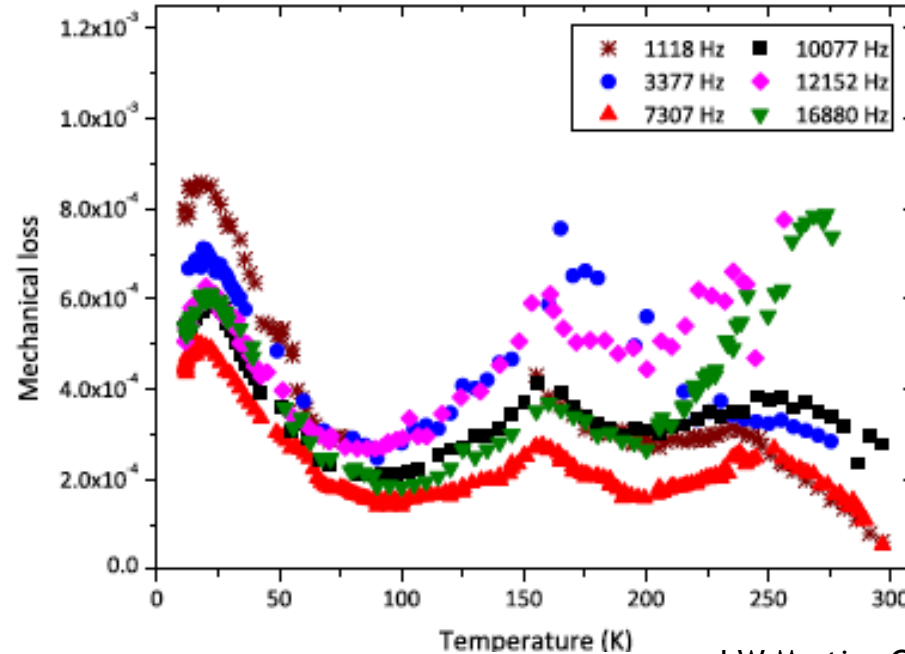
9/18/2015



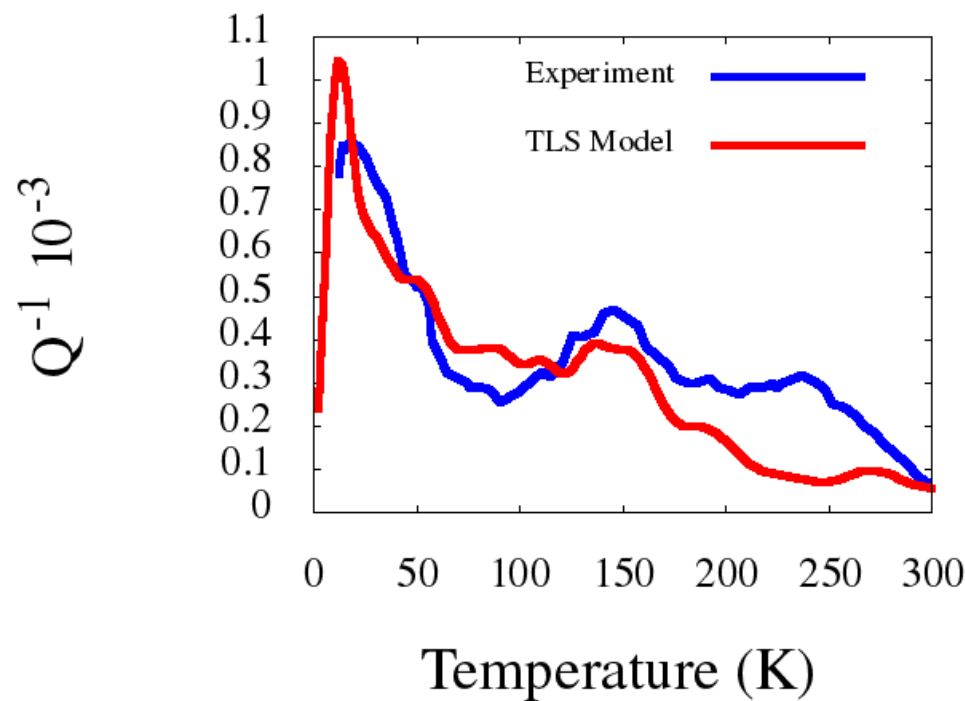
<http://www.ligo.org/science/GW-Sources.php>



<http://10m-prototype.aei.uni-hannover.de/design-and-sensitivity>



I W Martin, *Class. Quantum Grav.* 2014.



# Outline

- Describe Theory (W. A. Phillips *Rep. Prog. Phys.* 1987)
  - Introduce two-level systems (TLS)
  - Find the susceptibility
  - Calculate the internal friction
- Describe Model: Classical molecular dynamics (MD)
- Apply the model to Ta<sub>2</sub>O<sub>5</sub> and SiO<sub>2</sub>
- Conclusion

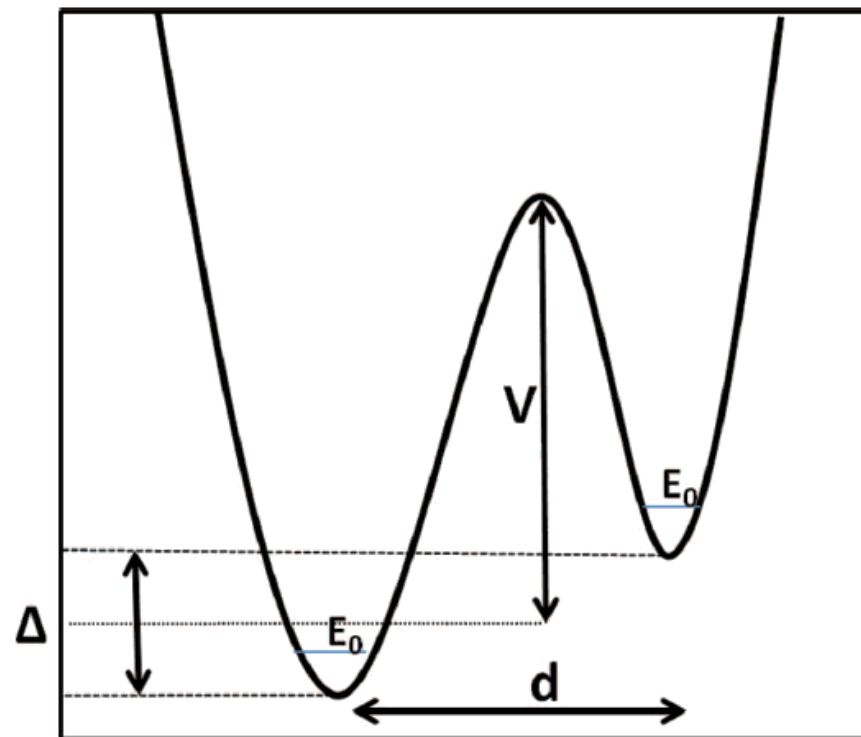
# Two-Level System: The Basics

- Let's start by examining a two-level system (TLS). The Hamiltonian of the system is:

$$H = H_1 + (V - V_1) = H_2 + (V - V_2),$$
 where  $H_i$  is the Hamiltonian of isolated well  $i$ , and  $V_i$  is the potential of that well.

- Assume that the asymmetry is caused by coupling to an electric or mechanical field.
- In a localized representation, where  $\varphi_i$  and  $E_i$  are the harmonic oscillator wave function and energy in well  $i$ , the Hamiltonian is:

$$H = \begin{vmatrix} E_1 + \langle \varphi_1 | V - V_1 | \varphi_1 \rangle & \langle \varphi_1 | H | \varphi_2 \rangle \\ \langle \varphi_2 | H | \varphi_1 \rangle & E_2 + \langle \varphi_2 | V - V_2 | \varphi_2 \rangle \end{vmatrix}$$



Rashid Hamdan, *J. Phys. Chem* 2014.

# Two-Level System: The Basics

- We can diagonalize this Hamiltonian, and we obtain two states with

$$E = \pm E/2 = \pm 1/2 \sqrt{\Delta^2 + \Delta_0^2}:$$

$$\begin{aligned}\psi_1 &= \varphi_1 \cos\theta + \varphi_2 \sin\theta \\ \psi_2 &= \varphi_1 \sin\theta - \varphi_2 \cos\theta\end{aligned}$$

$$\text{Where } \tan(2\theta) = \frac{\Delta_0}{\Delta}.$$

- Note that when  $\Delta \gg \Delta_0$ ,  $\psi_1 = \varphi_1$ , and  $\psi_2 = \varphi_2$ .
- The other limit, when  $\Delta \ll \Delta_0$ , gives

$$\begin{aligned}\psi_1 &= 1/\sqrt{2} (\varphi_1 + \varphi_2) \\ \psi_2 &= 1/\sqrt{2} (\varphi_1 - \varphi_2)\end{aligned}$$

# Two-Level System: Electric Susceptibility and Dipolar Relaxation

- Using the relaxation time approximation for the population difference, and assuming a wave of the form  $\xi(t) = \xi_0 e^{-i\omega t}$ , we get that the dielectric susceptibility is

$$\chi(\omega) = \frac{\chi(0)}{1 - i\omega\tau} = \frac{\bar{\alpha}}{1 - i\omega\tau}$$

- To find the energy lost to this system of dipoles, we need to find the imaginary part of the susceptibility:

$$\chi''(\omega) = \frac{\omega\tau}{1 + \omega^2\tau^2} \bar{\alpha} = \frac{\omega\tau}{1 + \omega^2\tau^2} \frac{p_0^2}{3kT} \frac{\Delta^2}{E^2} \operatorname{sech}^2\left(\frac{E}{2kT}\right)$$

# Two-Level System: Mechanical Loss

- This leads to the total internal friction for the system:

$$Q^{-1} = \frac{1}{(3kT)\varepsilon} \iint d\Delta dV \frac{\omega\tau}{1 + \omega^2\tau^2} \gamma^2 \operatorname{sech}^2\left(\frac{\Delta}{2kT}\right) N(\Delta, V)$$

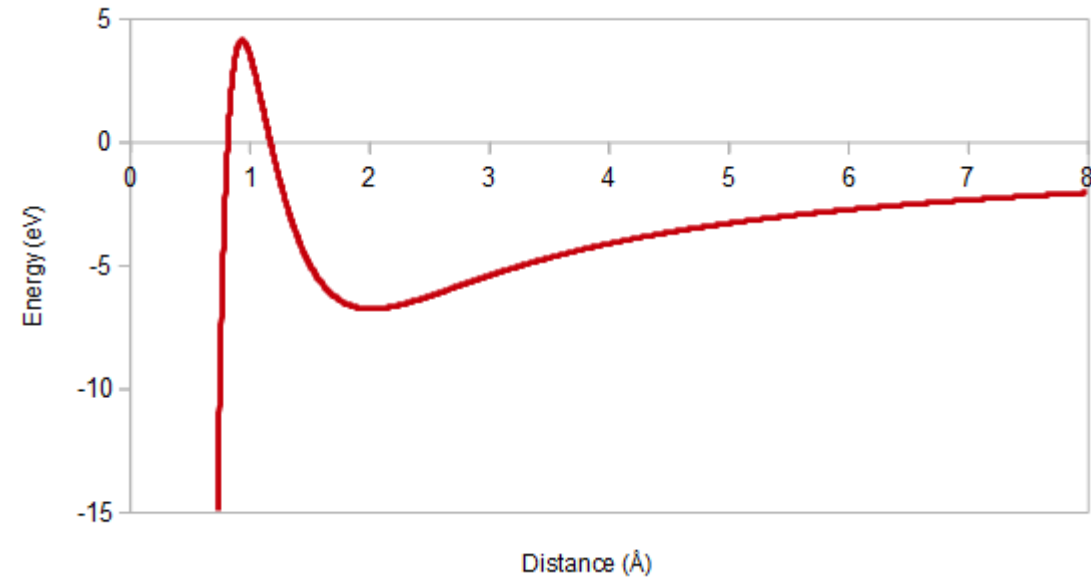
where

- $N(\Delta, V)$  is a number density of TLS's
- $\gamma$  is the mechanical dipole
- $\tau$  is the relaxation time
- $\omega$  is the angular frequency of the wave
- $\varepsilon$  is the Young's modulus for the system

# Classical MD Basics

- Classical description of forces:
  - Built on  $F=ma$
  - Interatomic potentials are modeled to fit experimental data (Density, elastic moduli, radial distribution functions, etc.)
  - Potentials were developed by Jonathan Trinastic.

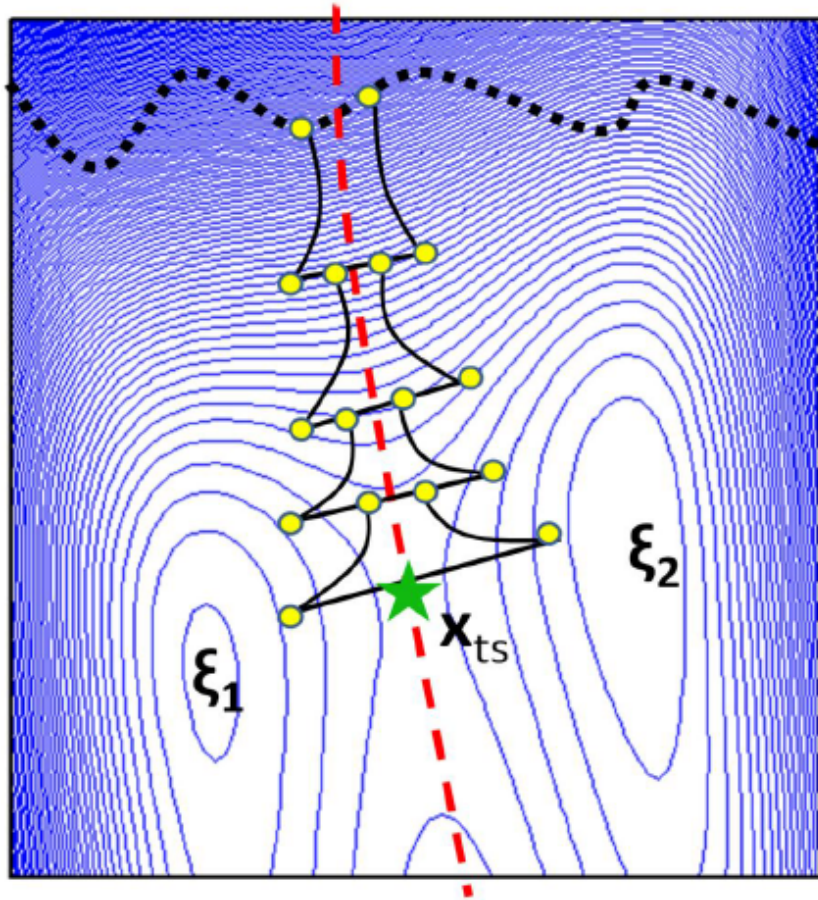
$$V_{1-2}(r) = Ae^{-Br} - \frac{C}{r^6} + \frac{kq_1q_2}{r^2}$$



[https://en.wikipedia.org/wiki/Buckingham\\_potential](https://en.wikipedia.org/wiki/Buckingham_potential)



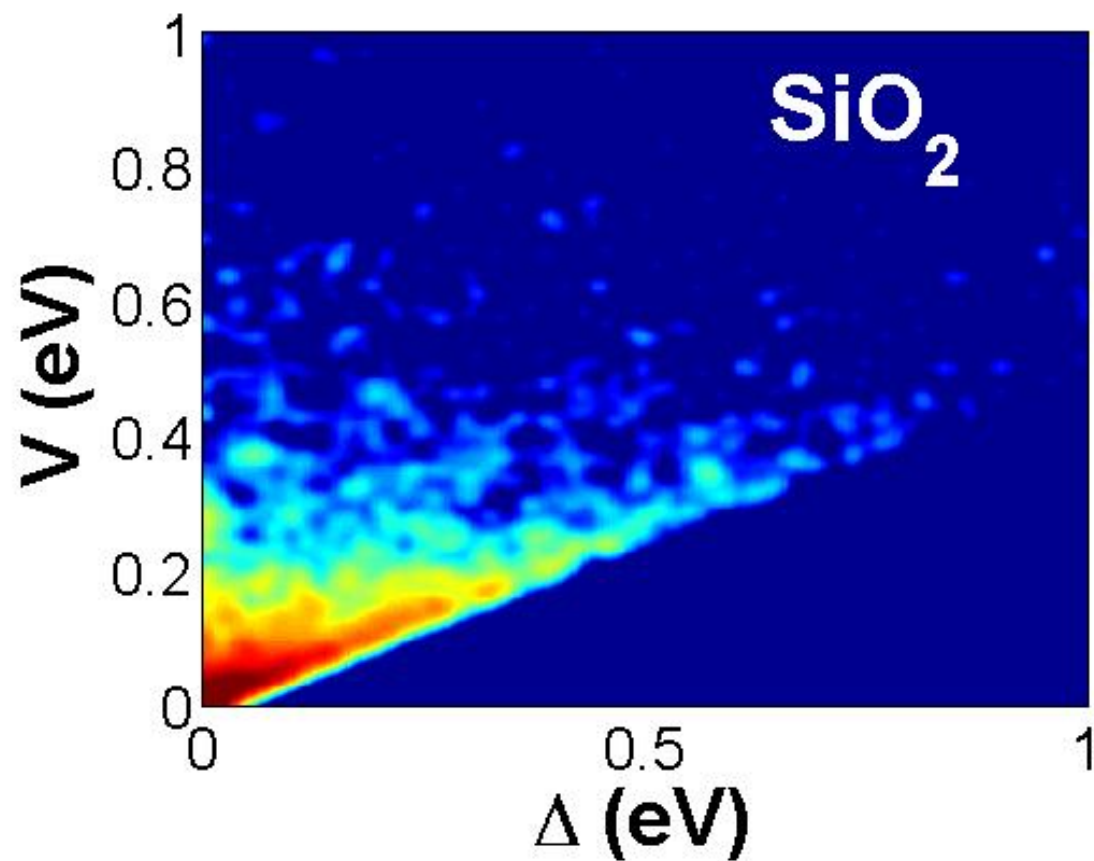
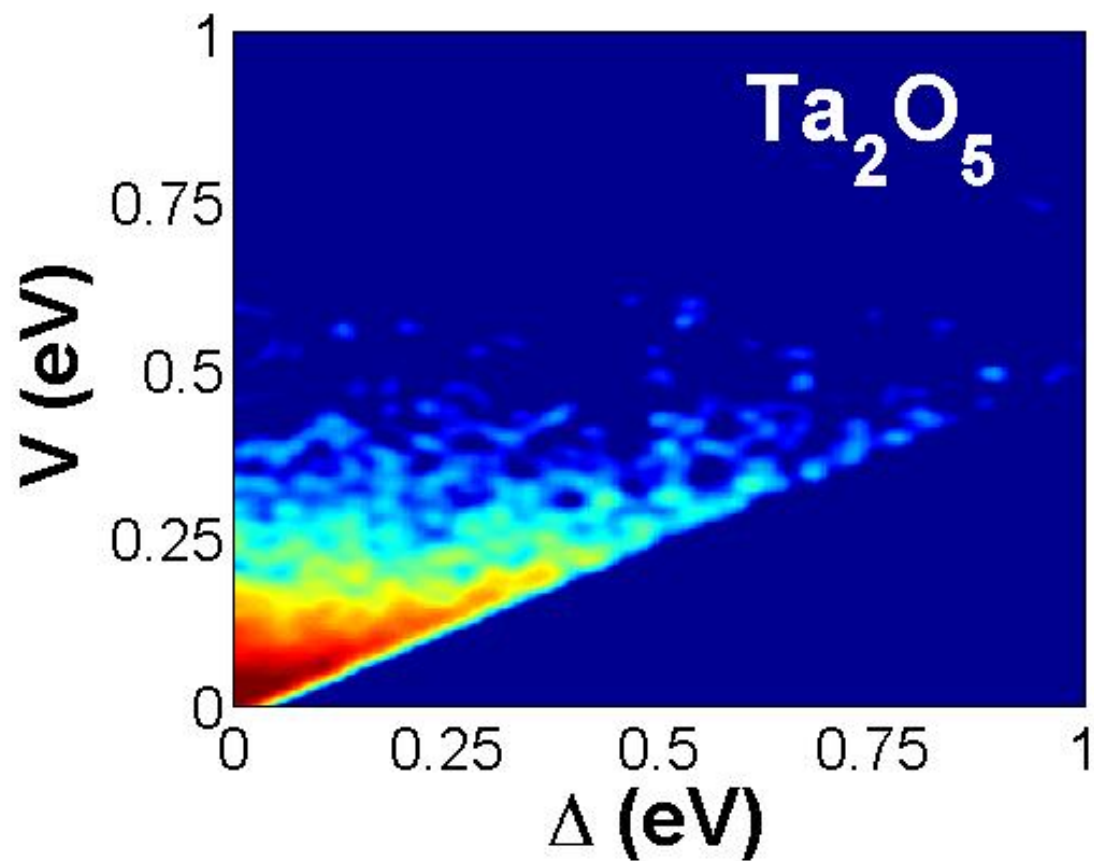
# The TLS model in MD



Rashid Hamdan, *unpublished*.

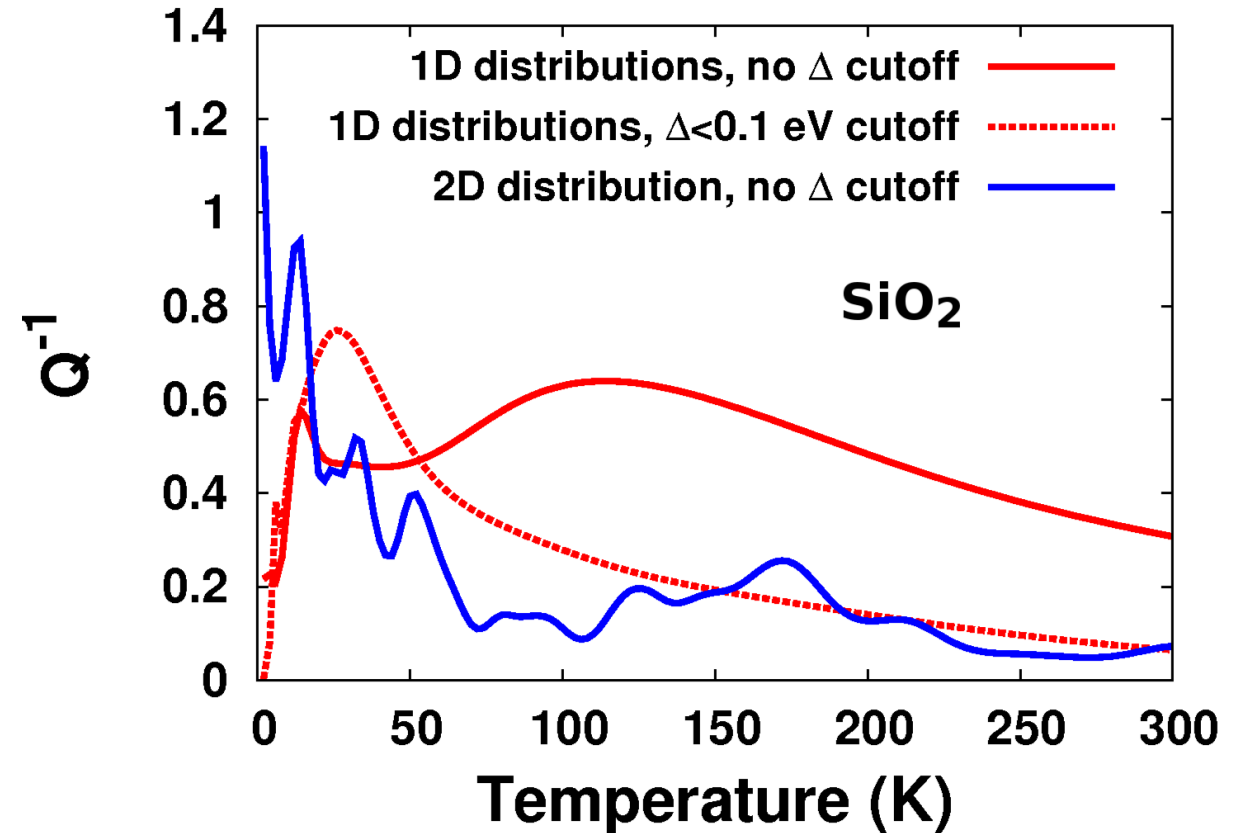
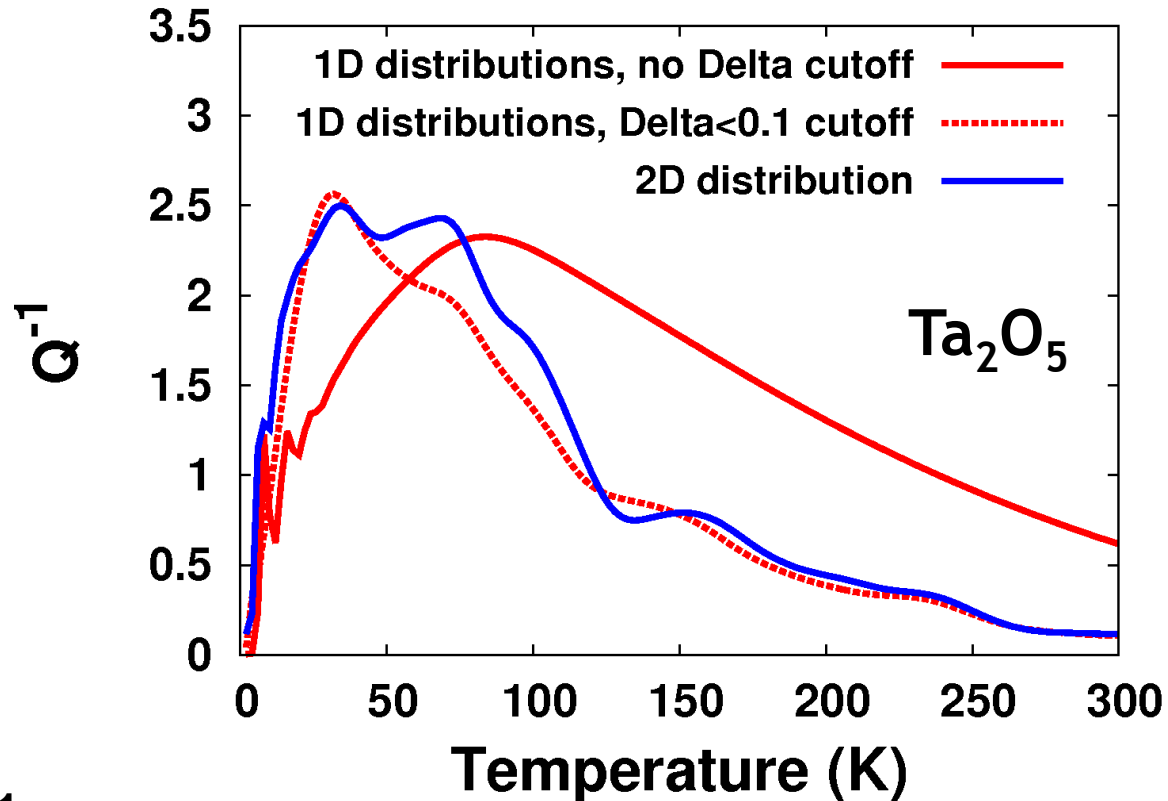
- We do this method thousands of times, to get  $N(\Delta, V)$ .
- We calculate the average relaxation time and average coupling constant from a subset of these TLS's

# Model Inputs: TLS Distribution

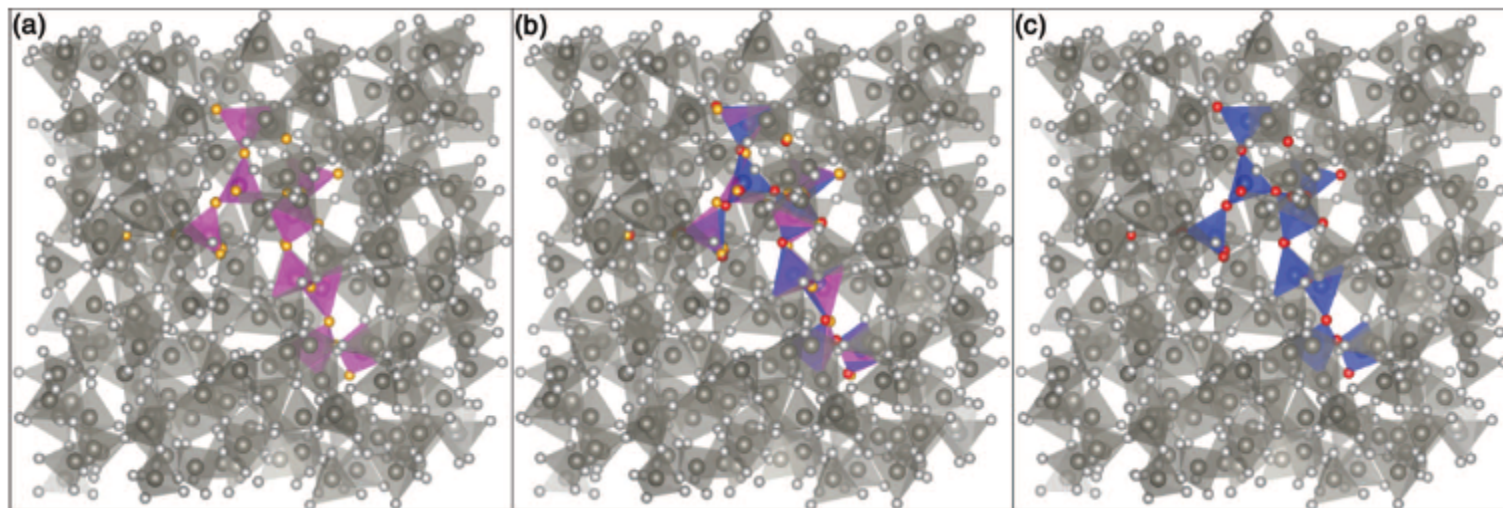


# Mechanical Loss: Approximations

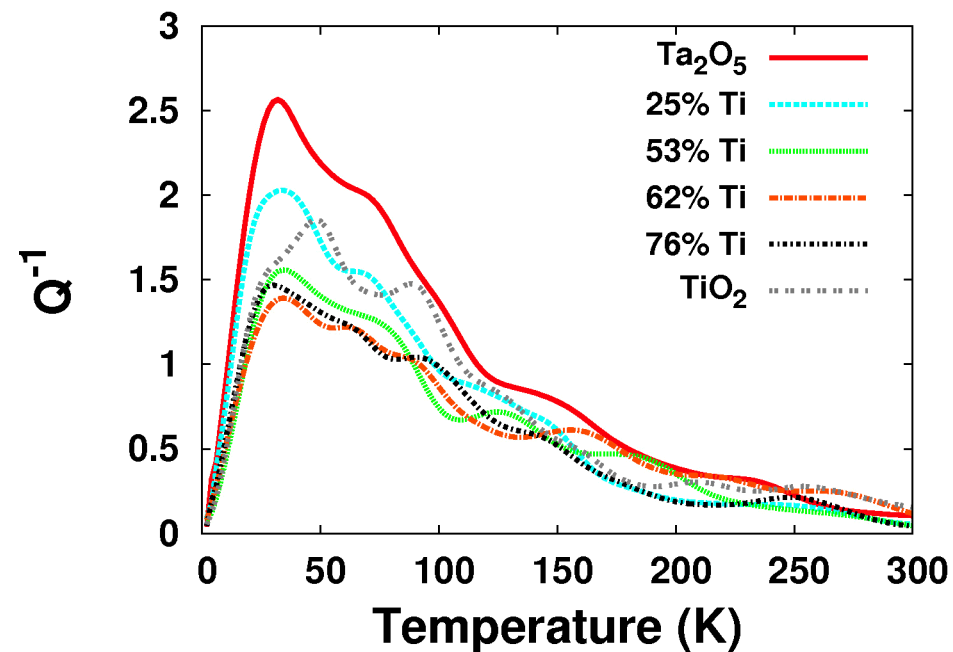
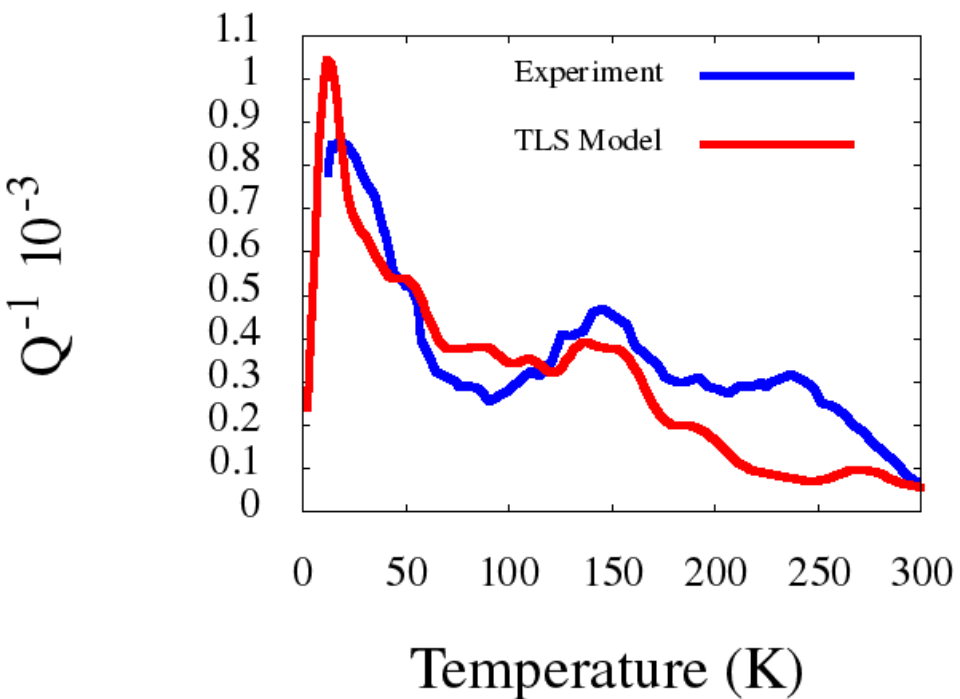
- Asymmetry Cut-off
  - Previously, a 0.1 eV asymmetry cut-off was used to better match



# What our model contributes



Rashid Hamdan, *J. Phys. Chem* 2014.



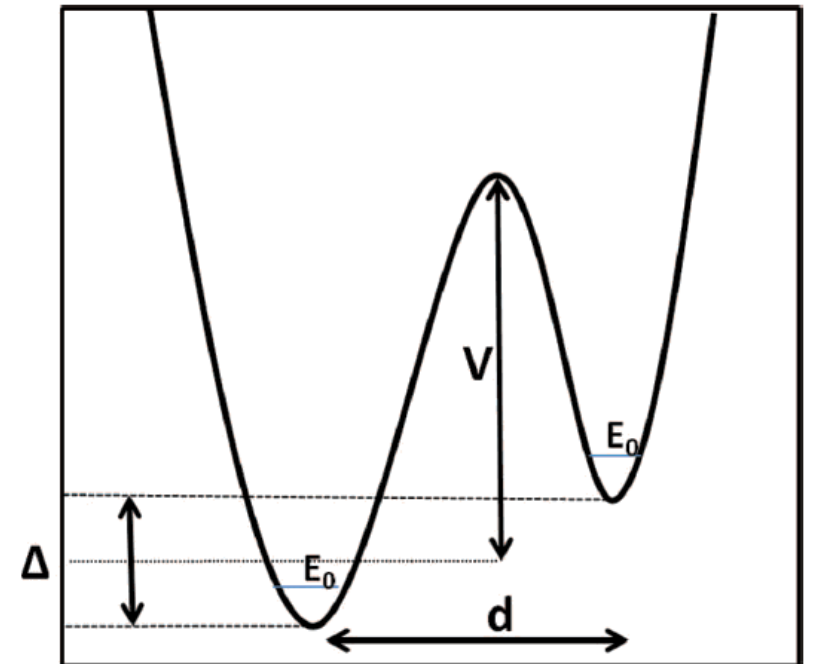
# Conclusion

- The acoustic loss in amorphous solids is a consequence of applying a mechanical field to systems of dipoles, and can be derived from a model Hamiltonian where we assume two-level systems where symmetry is broken by an applied field.
- Using classical molecular dynamics to provide inputs for the TLS model gives good agreement with the low temperature peak. Using the 2-D distribution, more detailed features can be seen at higher temperature.
  - For  $\text{SiO}_2$  this shows a second peak at 150K which matches experiment.
  - For  $\text{Ta}_2\text{O}_5$ , it does not lead to a better description but better statistics may be required.
- This allows us to
  - Understand the atomic transitions that cause internal friction
  - Predict internal friction under different doping
  - Determine what causes higher temperature peaks



# Model Inputs: Elastic Moduli and Coupling

- Young's modulus
  - $\sigma_i = c_{ij}\varepsilon_i$
  - Strain the system to determine what the elastic moduli are. To compare to mechanical loss experiments, we are interested in longitudinal modes, so we need the Young's modulus.
- Coupling Constant
  - $\gamma_j = 1/2 \frac{\partial \Delta}{\partial u_j}$
  - The asymmetry changes as unit cell is strained, which is the coupling to mechanical field.



# Model Inputs: Relaxation Time

- The relaxation time is calculated using the Arrhenius law:

$$\tau = \tau_0 e^{\frac{V}{kT}} \operatorname{sech}\left(\frac{\Delta}{2kT}\right)$$

and is averaged over all TLS's found.

- In the Arrhenius law, the shape of the well changes the attempt frequency, which is inversely related to  $\tau_0$ . This value is calculated for each TLS by

$$\tau_0^{-1} = \frac{\prod_{i=1}^{3N} \nu_i^0}{\prod_{i=1}^{3N} \nu_i^s} e^{S/k}$$

where  $\nu_i^0$  are the vibrational frequencies at the minimum,  $\nu_i^s$  are the vibrational frequencies at the saddle point. The exponential represents the entropy term, as a single well may be a part of many different TLS's.