Modeling of fused silica optics and coatings

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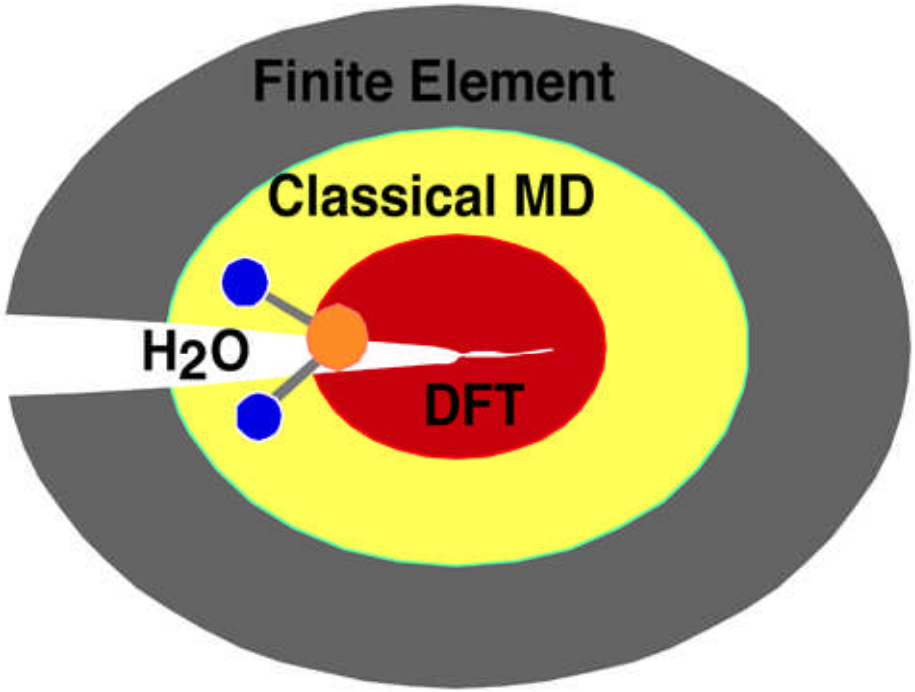
Multi-scale simulation of material behaviors including chemical reactions



- Thermal Noise, Mechanical loss: A serious problem from the LIGO pr
- Crack propagation and hydrolytic weakening in SiO_2
- Chemo-mechanical processes

Quantum modeling for materials properties

Density functional theory with general gradient approximations: A state-of-the-art method for first-principles material simulation with chemical accuracy

The Kohn-Sham equation for a system with periodic boundary condition is written as follows,

$$\left[-\frac{1}{2}\nabla^2 + V\left(\rho(r)\right)\right]\psi_\alpha = \varepsilon_\alpha \psi_\alpha ; \alpha = (n, \vec{k})$$

$$V(\rho) = V_{e-nuc} + V_H(\rho) + V_{XC}(\rho)$$

~10^3 electrons

$$\psi_\alpha(r) = \psi_{n,k}(r) = \sum_{\vec{G}, \frac{1}{2}|\vec{G}+\vec{k}|^2 \le E_{cut}} c_{n,\vec{G}+\vec{k}} e^{i(\vec{G}+\vec{k})\vec{r}} \quad \text{or} \quad \psi_\alpha(r) = \psi_{n,k}(\vec{r}) = \sum_\mu c^k_{\mu n} \phi^k_\mu(\vec{r}) e^{i\vec{k}\cdot\vec{r}}$$

Molecular dynamics (MD) method

$$m_i \frac{d^2 \boldsymbol{R}_i}{dt^2} = -\nabla_{\boldsymbol{R}} U\left(\{\boldsymbol{R}\}, \rho(\boldsymbol{r})\right)$$

R: Nuclei position, ρ electron density, in general, one solve the whole wave function to get energy and forces. In classical MD, we replace U by empirical functions

Van Beest, Kramer, van Santen (BKS) Potential for SiO_2

PRL **64**, 1955 (1990)

$$U_{MD}\left(\{\mathbf{r}_{ij}\}\right) = \sum_{i<j} V_{ij}\left(\mathbf{r}_{ij}\right)$$

$$V_{ij}\left(\mathbf{r}_{ij}\right) = \frac{q_i q_j}{r_{ij}} + A_{ij} e^{-b_{ij} r_{ij}} - \frac{C_{ij}}{r_{ij}^6}$$

Classical MD
~10^6 -10^8 atoms
~nano-seconds
Good for obtaining statistics, but accuracy is limited by energy functions

A, b, C, q: potential parameters for Si-Si, O-O, & Si-O

Modeling and Simulation -- What we can do and what to expect

- Quantum Modeling -- based on density function theory
  Electronic Properties: **Energy barriers, dielectric functions, Young's modules, Poisson ratio,** effects of dielectric doping, parameters for
  classical simulations,

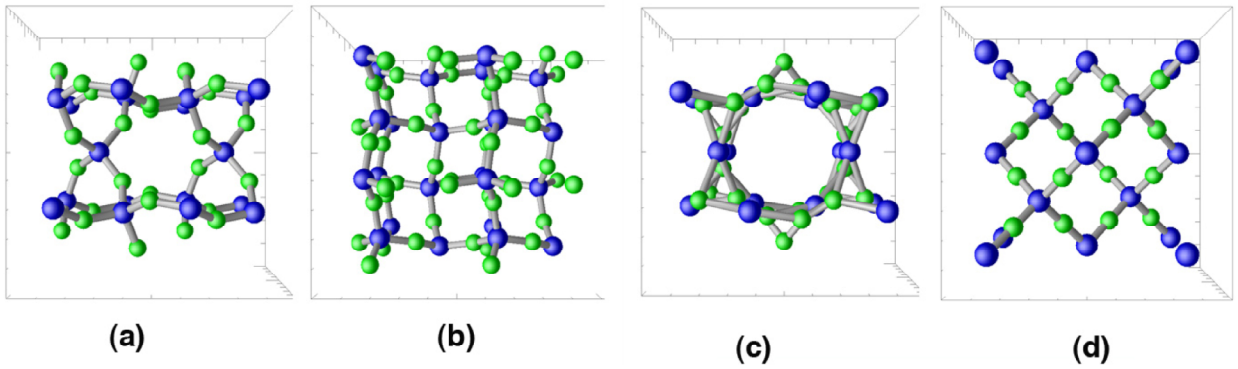
- Classical molecular dynamics
  Mechanical and thermodynamical properties, structure: **Young's modulus, Poisson ratio, thermal expansion coefficient, thermal conductivity**

- New development: Hybrid Quantum-classical simulation
  Embedding a quantum model cluster in a classical environment for better description of energy barriers.

- Challenges: Accuracy in energy barrier, quality of classical potential

Quantum calculation of crystal properties

	α-quartz	α-cristobalite	β-quartz	β-cristobalite
a (•) EXPTL	4.92	4.96	5.00	
a (•) SIESTA	5.02	4.93	5.18	
a (A) PWSCF	5.06	5.13	5.13	
c/a EXPTL	1.10	1.39	1.09	
c/a SIESTA	1.10	1.41	1.09	
c/a PWSCF	1.11	1.40	1.09	
E_c (eV/SiO_2) EXPTL	19.23	19.20	19.18	
SIESTA	21.34	21.30	21.29	21.13
VASP				
PWSCF				



(a)-(d)
α–quartz,
α-critobalite,
β-quartz
β–
cristobalite.

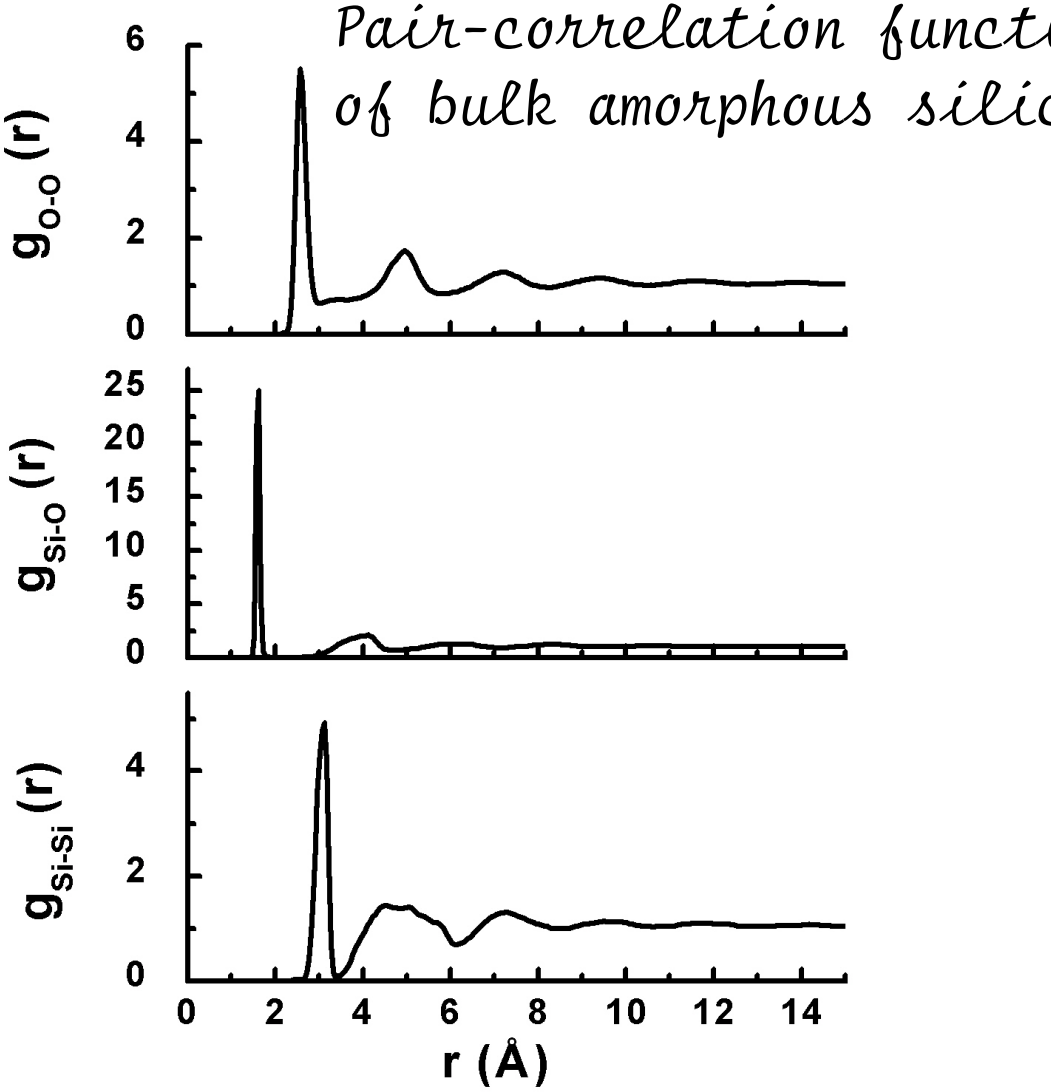
Amorphous silica

- The amorphous silica bulk is obtained by annealing of the liquid glass from 8000K to 300K.

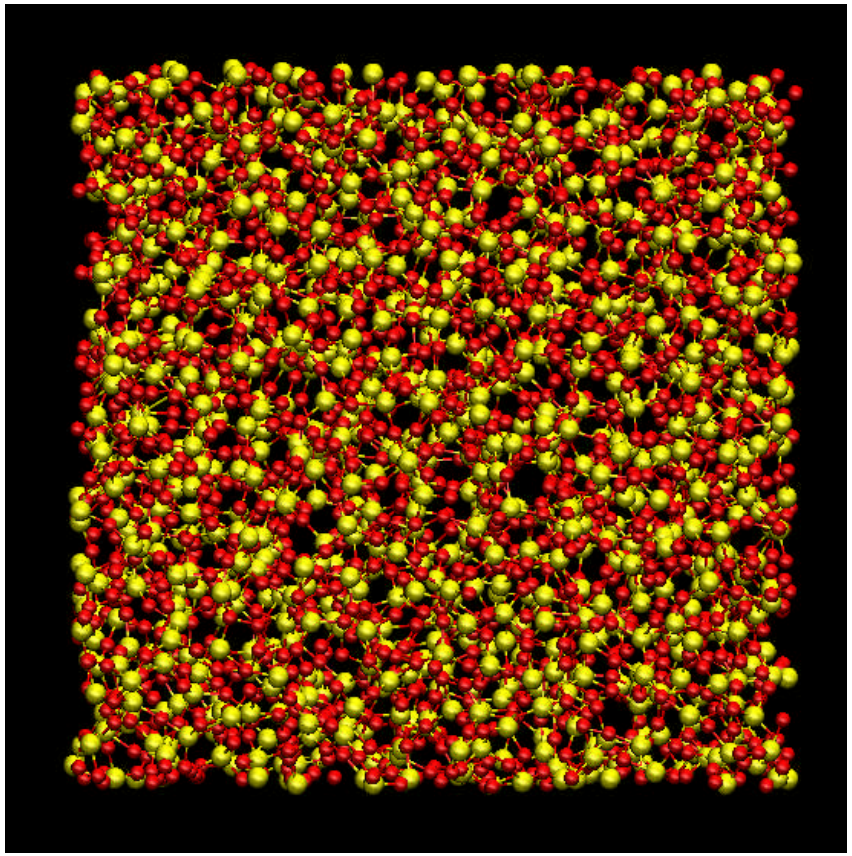
Huff et al, J. Non-Cryst. Solids **253**, 133 (1999)

- A 10^4-atom slab is used to simulate the surface.
- Density, pair-correlation functions are in agreement with experimental data

Wright J. Non-Cryst. Solids,



Properties of amorphous silica surfaces



- In the absence of strain, the Si-O bonds are inert to H_2O and NH_3, etc.
- Strained Si-O bonds greatly increase the reactivity by creating acidic and basic adsorption sites on silicon and oxygen.
- Reactive sites (surface defects) play crucial roles in the surface corrosion
- Two-membered-ring (TMR) is a surface defect with high abundance

Water destroys TMR, heating above 500 °C restores the TMR, surface dehydroxylation

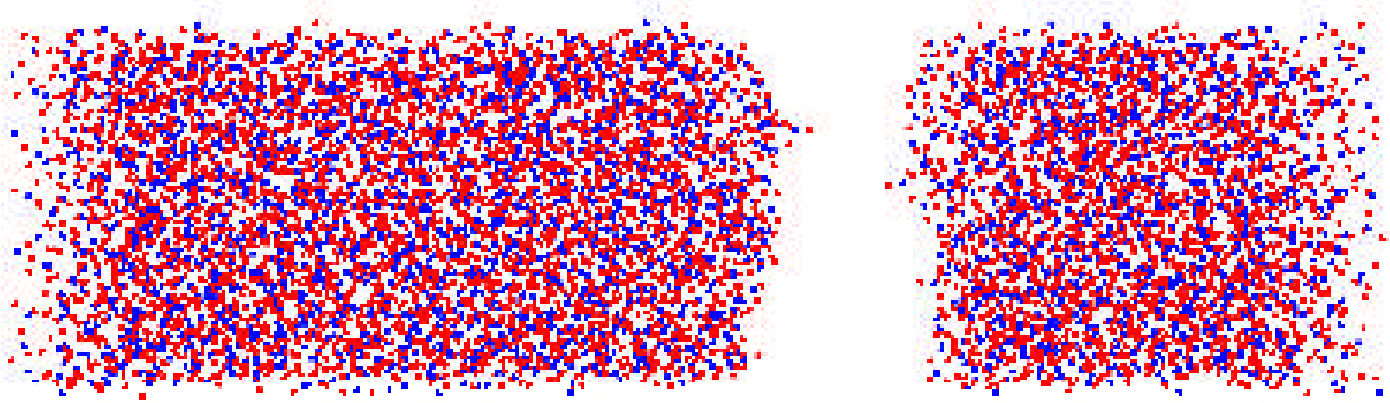
Bunker et al, Surf. Sci. 222, 95 (1989); Bunker et al, Surf. Sci. 210, 406 (1989)

Walsh et al, JCP 113, 9191 (2000); cluster model

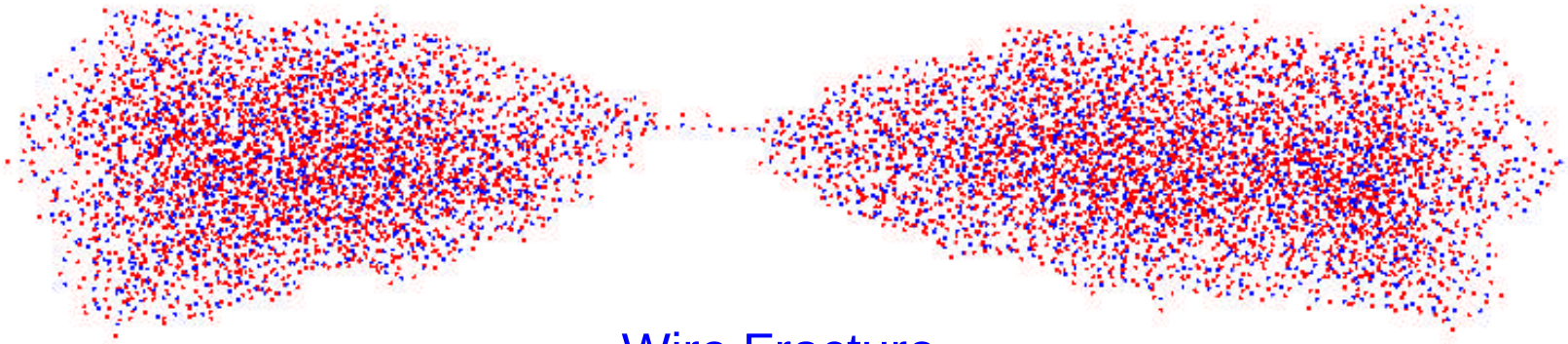
S. Iarori et al, JPC B105, 8007 (2001) β-cristobalite model

Results: Fracture Point Snapshot

Comparison between amorphous systems



Bulk Fracture



Wire Fracture

The Problem related to LIGO: Coating Thermal Noise

Relaxations of glasses affect:

- Neutron and light scattering
- Sound wave attenuation
- Dielectric loss

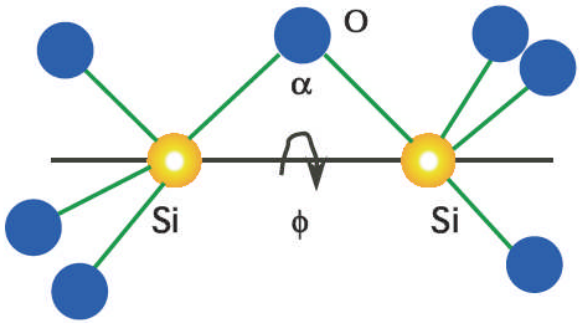
A direct relation between a microscopic quantity *V* and a macro-scopic measurement X'' is (Wiedersich et al. PRL (2000) 2718

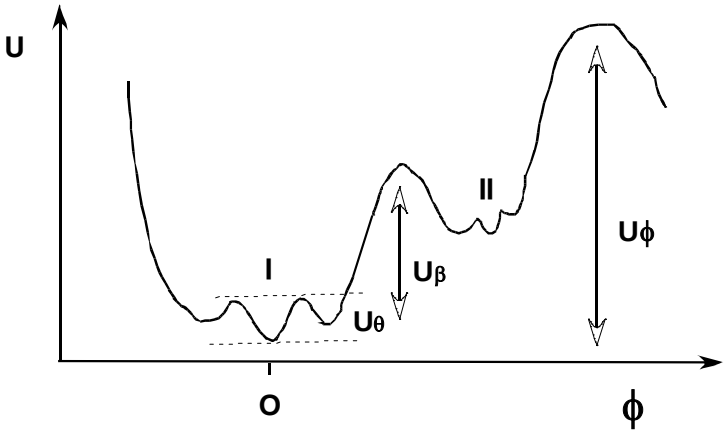
$$\chi''(\nu) \propto Q^{-1} \propto \int_0^{\infty} \frac{2\pi\nu\tau}{1+(2\pi\nu\tau)^2} g(V)dV$$

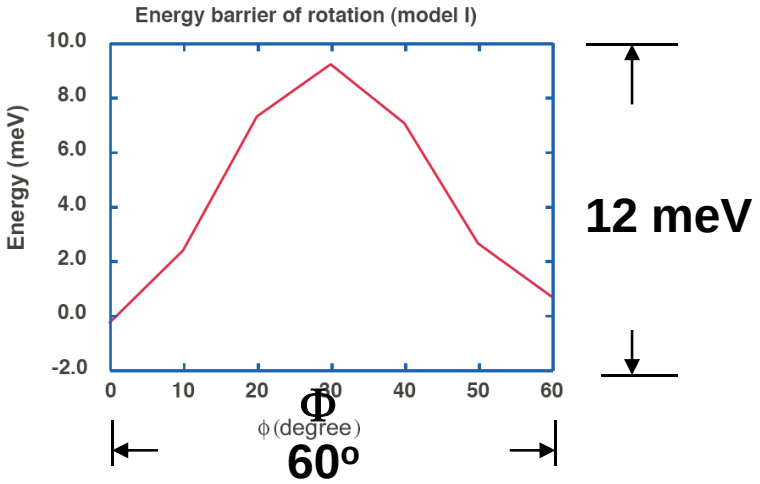
$\chi''(\nu)$: light scattering scattering susceptility,
V: barrier, Q^{-1}: internal friction
$g(V)$: barrier distribution, τ: relaxation time

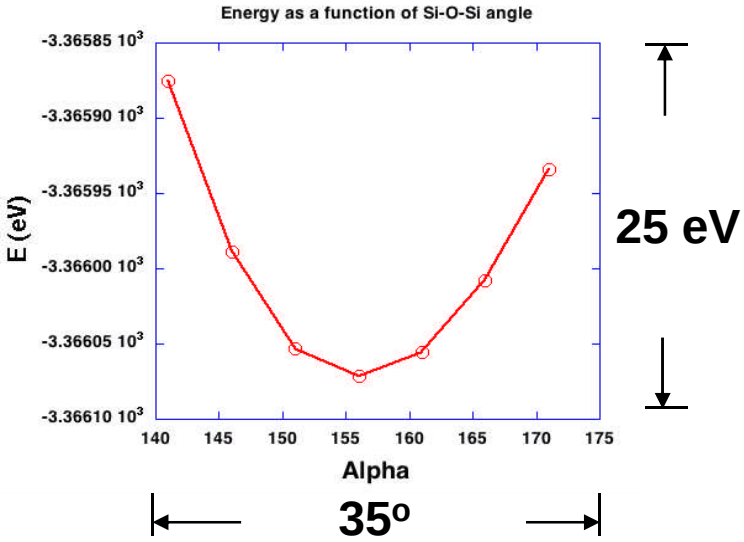
Thermal noise relates to *Q* via Young's modules, Poisson ratio,… G. Harry et al. Class Quantum. Grav. 19 (2002) 897-927 ***Recent reference****: G.Harry talk in* LIGO/Virgo Thermal Noise Workshop October 2006

Quantum calculations of silica



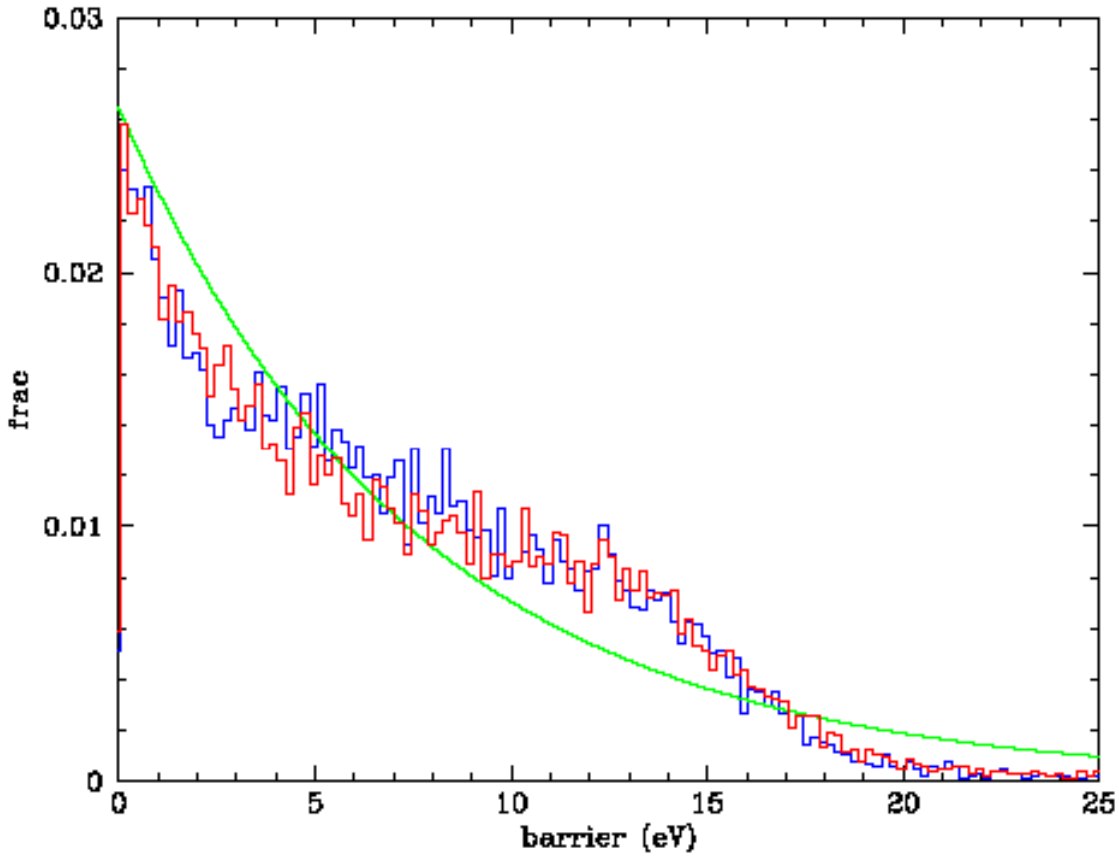






M.R. Vukcevich, J. Non-Crystl. Solids
Vol. 11 (1972) pg.26-63
C.M. Bartenev, et al. Inorganic Materials
Vol.32, No.6 (1996) pg.671-682

Barrier distribution from classical MD



Blue: Bulk
Red: Surface

Green:

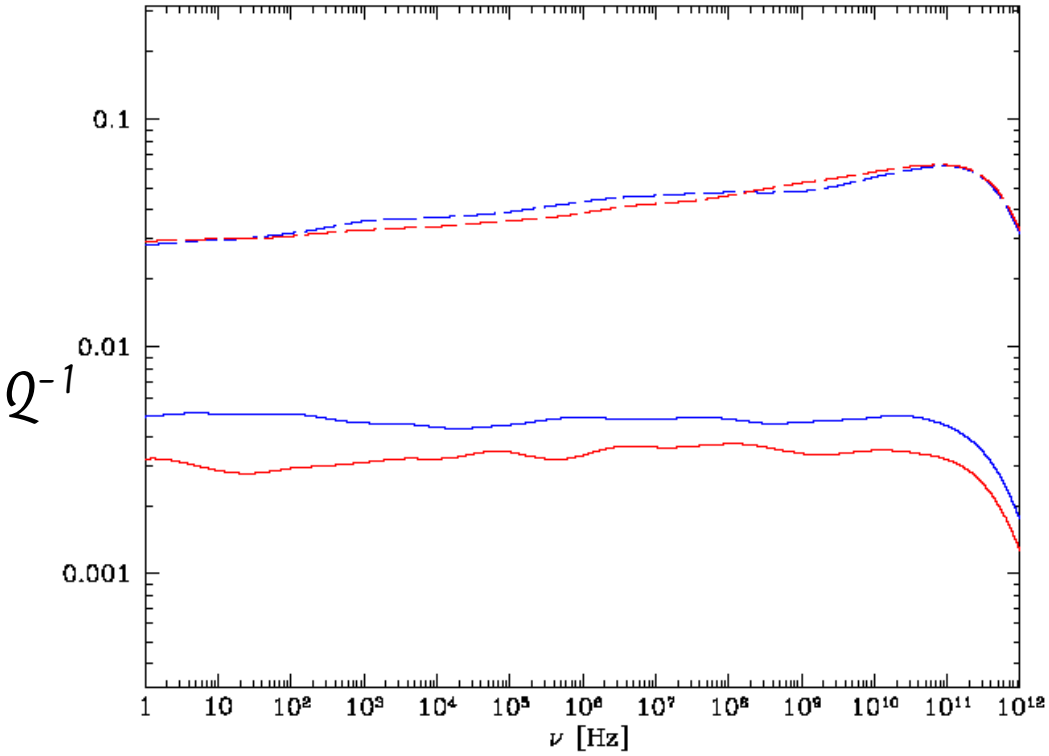
$$g(V) = V_0^{-1} \exp(-V / V_0)$$

$$V_0 \approx 8eV$$

~319 $k_B T$

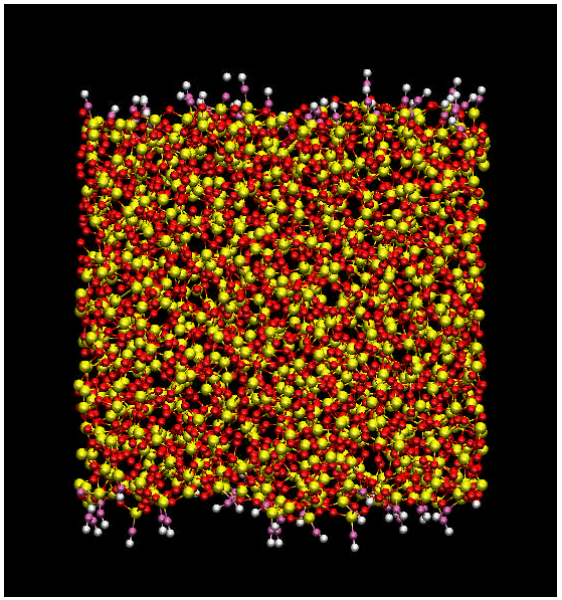
Wiedersich et al.
84, 2718, PRL (2000)

Calculated Q^{-1} vs. frequence



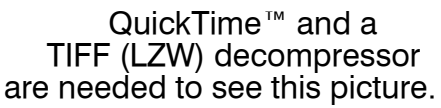
Solid: 300 K
Dashed: 32x300 K
Blue: Bulk
Red: Surface

Conclusion:
Bad compared to experiments!



Improvements
Relaxation during barrier calculation
Locating all possible low barriers
Improving potential energy function
Improving statistics
Also: Investigate hydroxylated surfaces

Ta_2O_5: Structure



A high-temperature structure for Ta_2O_5 with modulations by TiO_2 substitution

Makovec *et al.* Journal of Solid State Chemistry 179 (2006) 1782–1791

PLAN: quantum calculations of Ta_2O_5 + TiO_2

QuickTime™ and a
TIFF (LZW) decompressor
are needed to see this picture.

Optimized Ta_2O_5 high-temperature crystal structure (via DFT). High-T structure is closer to amorphous structure, a better model than the low-T one.

Structure and mechanical properties of pure and doped Ta_2O_5

Effect of local chemistry on Young's moduli, Poisson ratio

$$S_x(f) = 2k_B T \phi_{\text{eff}} (1-\sigma^2)/(\pi^{3/2} f w Y),$$

$$\begin{aligned}\phi_{\text{eff}} = \phi + d/(\sqrt{\pi} w Y_\perp)\big((Y/(1-\sigma^2) - 2\sigma_\perp^2 Y Y_\parallel / (Y_\perp(1-\sigma^2)(1-\sigma_\parallel)))\phi_\perp \\ + Y_\parallel \sigma_\perp (1-2\sigma)/((1-\sigma_\parallel)(1-\sigma))(\phi_\parallel - \phi_\perp) \\ + Y_\parallel Y_\perp (1+\sigma)(1-2\sigma)^2 / \big(Y(1-\sigma_\parallel^2)(1-\sigma)\big)\phi_\parallel\big),\end{aligned}$$

G. Harry et al. Class. Quantum Grav. 24 (2007) 405–415

Simulation Milestones

- Examine properties of silica using the current model and compare with existing experimental measurement on SiO_2 bulk and surface, extend our investigation to silicates. (Advance LIGO)

- Investigate the effects of coating and dopant materials used in the LIGO experiment, and understand the change of physical properties. (Ta_2O_5, TiO_2, HfO_2,Nb_2O_5,..titania, zirconia lutetium doping…) (Advance LIGO)

- In collaboration with experiments, seek for new coating materials that have optimal combinations of low thermal noise and optical absorption, computer-aided material design (beyond Advance LIGO).

Collaborators

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