Progress and Plans in Optical Coating Research

LIGO-Dawn Workshop II

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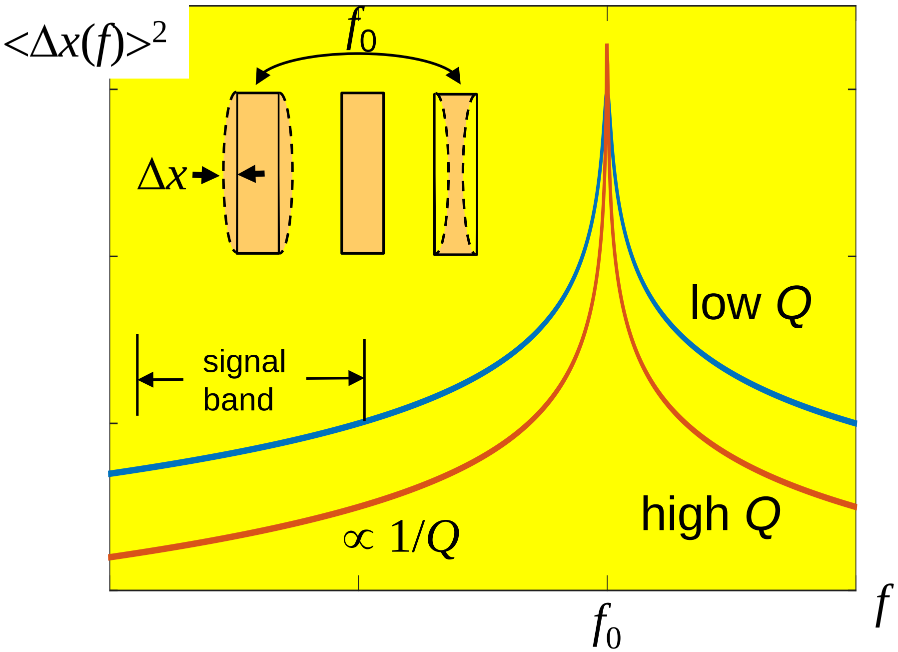
Brownian Thermal Noise in LIGO Mid-Band



Oversimple: kT of energy per elastic mode

uniform mass, viscous damping

– moves front of mirror w.r.t. center of mass

Coating-dominated loss
structural damping:

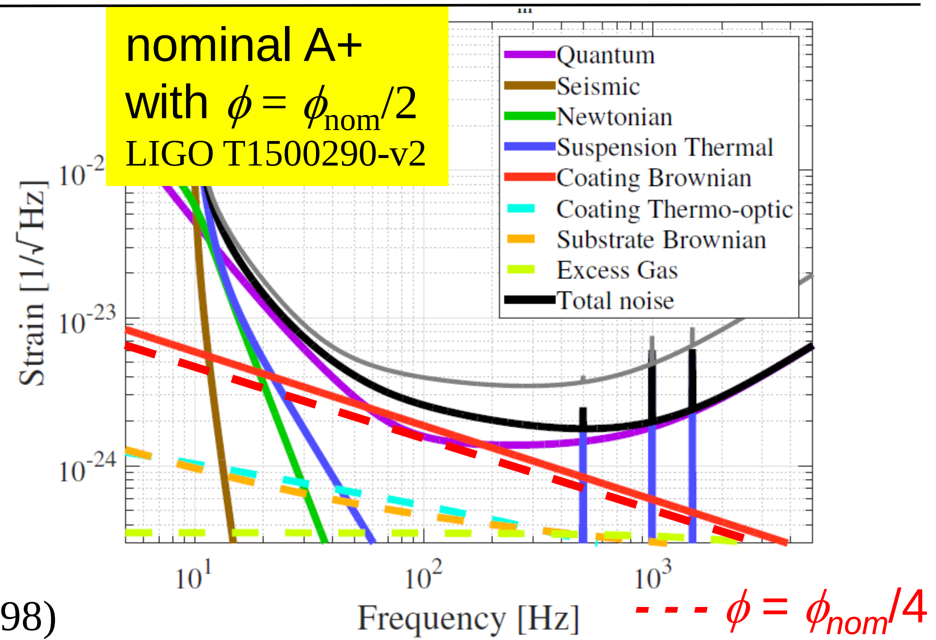
coating elastic loss

coating thickness

$$S_x(f,T) \approx \frac{2k_BT}{\pi^2 f}\frac{d}{w^2Y}\phi\left(\frac{Y'}{Y}+\frac{Y}{Y'}\right)$$

beam radius

Y Levin *Phys. Rev. D* **57** 659 (1998)



Plausible A+ Goals

$$\phi_{\mathrm{TiO_2:Ta_2O_5}} = 2\times10^{-4}$$
$$\phi_{\mathrm{SiO_2}} = 4\times10^{-5}$$

- A-LIGO
  - optimized Ti:Ta_2O_5/SiO_2 mirrors

- A+ LIGO
  - improve elastic dissipation by 2 – 4 x

    room temperature $\phi < 1\mathrm{x}10^{-4}$

- While maintaining optical properties over 34 cm diameter

  at 1.06 μm for A+-LIGO
  - optical absorption: ~0.5 ppm
  - micro-roughness scatter: ~1 ppm
  - uniformity: ~0.5 nm

- A+ timeline:
  - coating pathfinder begins optimistically 15 months from now

    funding might delay ~ 1-2 years

Outline

- Quick sketch of what we (think we) know
- Two-level system (TLS) model for internal friction
- Theoretical guidance
  - molecular dynamics
- More theory
  - "Ultra-stable glasses" from high-temperature deposition
- Amorphous silicon
  - model system for ultra-stable glass
  - potential material for LIGO Voyager
- Structural characterization
- Some thoughts on strategy going forward

somewhat more detail in Fejer GWADW 2016, G1601192-v2

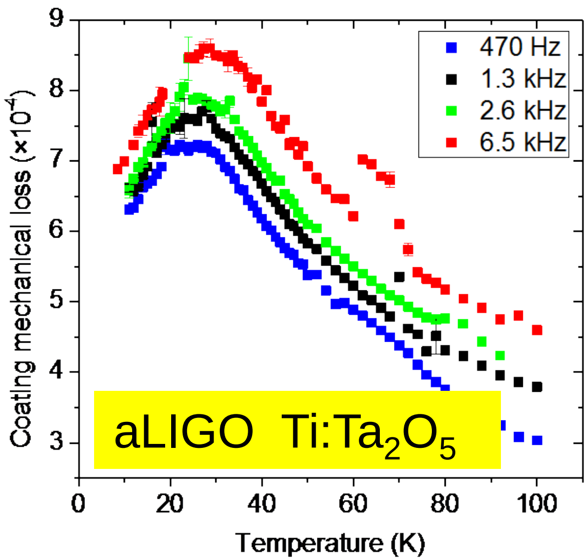
General Observations About Coating Elastic Loss

- Volume rather than interface losses dominate in tantala/silica mirror

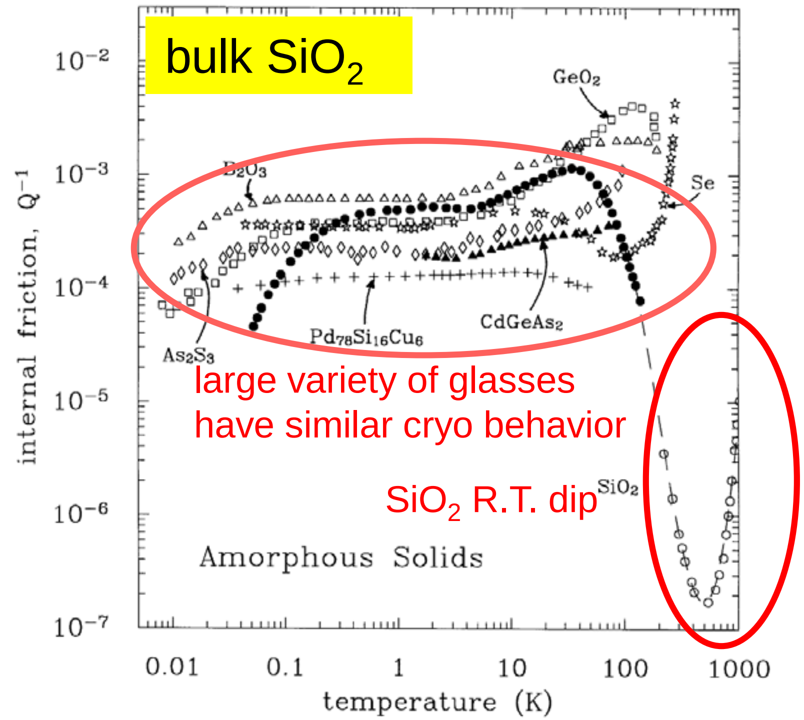
D. Crooks, Class. Quantum Grav. 23 (2006) 4953–4965

  – current values: Ti:tantala ~5x lossier than silica

- Typical behavior vs temperature and acoustic frequency
  – amorphous materials have loss peak at low temperatures



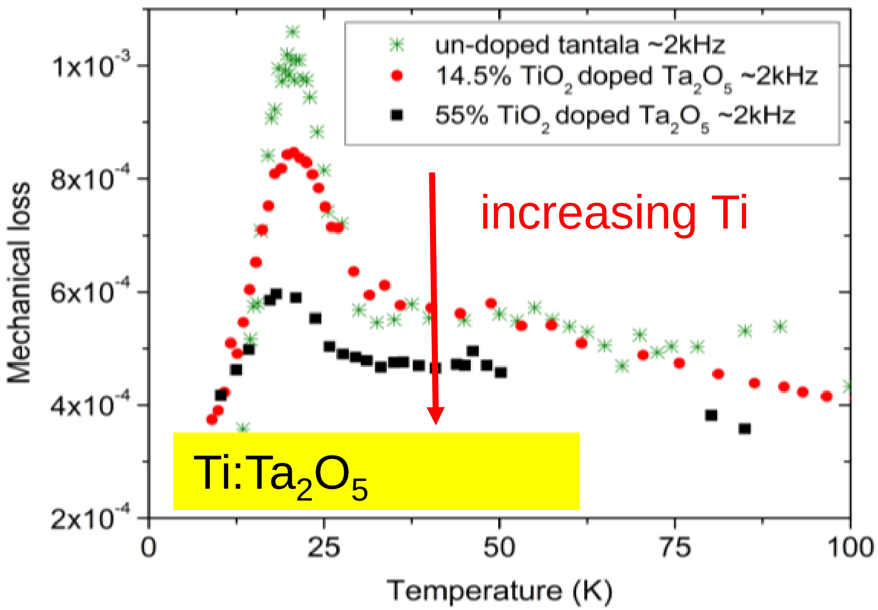
I W Martin et al, *Class. Quant. Grav.* **27** 225020, (2010)



K.A. Topp, *Z. Physik B Condensed Matter* **101** 235–45 (1996)

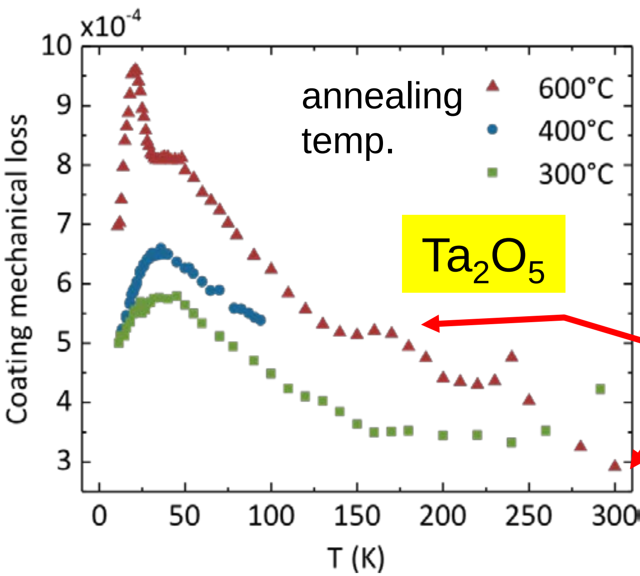
Doping and Annealing Alter Dissipation

- Loss modified by dopants
  - TiO_2 doping
    reduces losses in Ta_2O_5



P. Murray et al, U. Glasgow
LIGO-G1500874

- Annealing modifies loss spectra



annealing modifies behavior
can improve loss at some temperatures
while worsening it at others

[I W Martin et al, Class. Quant. Grav. 27 225020, 2010]

Find Better Amorphous Oxides?

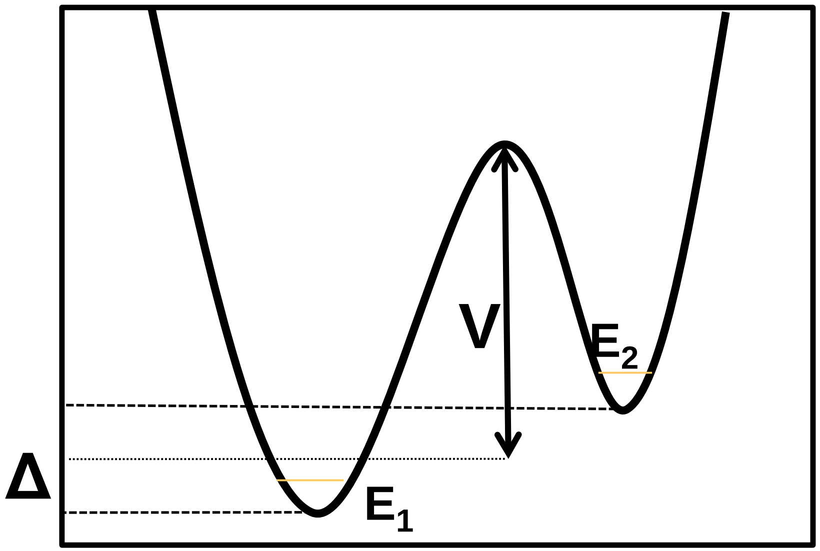
- Random search through ternary oxides?
  - thousands of host/dopant combinations
  - thermal processing adds another degree of freedom

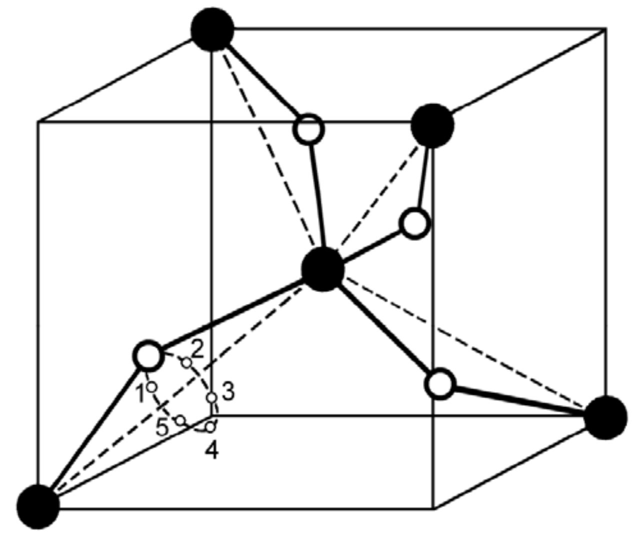
- *Ars longa, vita brevis*
  - Edisonian methods used to date may not scale gracefully
    - limited time and $$ available

- Understanding underlying mechanisms useful to guide experiment
  - two-level systems (TLS)
  - molecular dynamics modelling
  - “ultra-stable” glasses
  - atomic structure characterization

Low-frequency losses in amorphous dielectrics

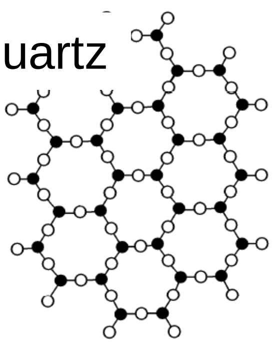
- Conventionally associated with low energy excitations (LEEs)
  - conceptualized as two-level systems (TLS)





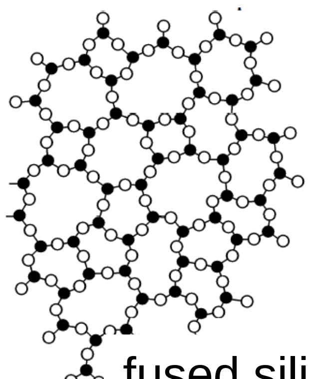
Oversimple picture: bond flopping

crystal quartz



(● = Si, ○ = O).

A)



fused silica

Distribution of TLS in silica due to disordered structure

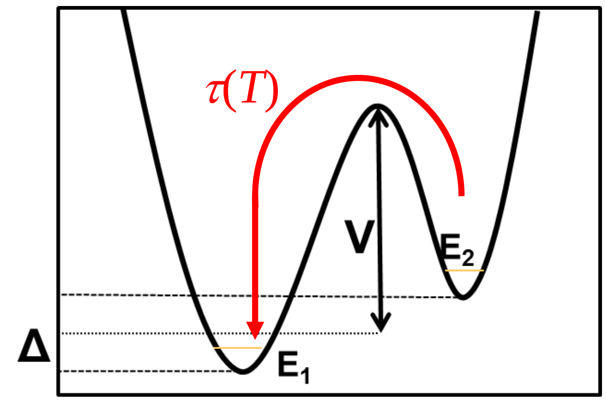
figures from B.S. Lunin monograph

Elastic Dissipation by TLS

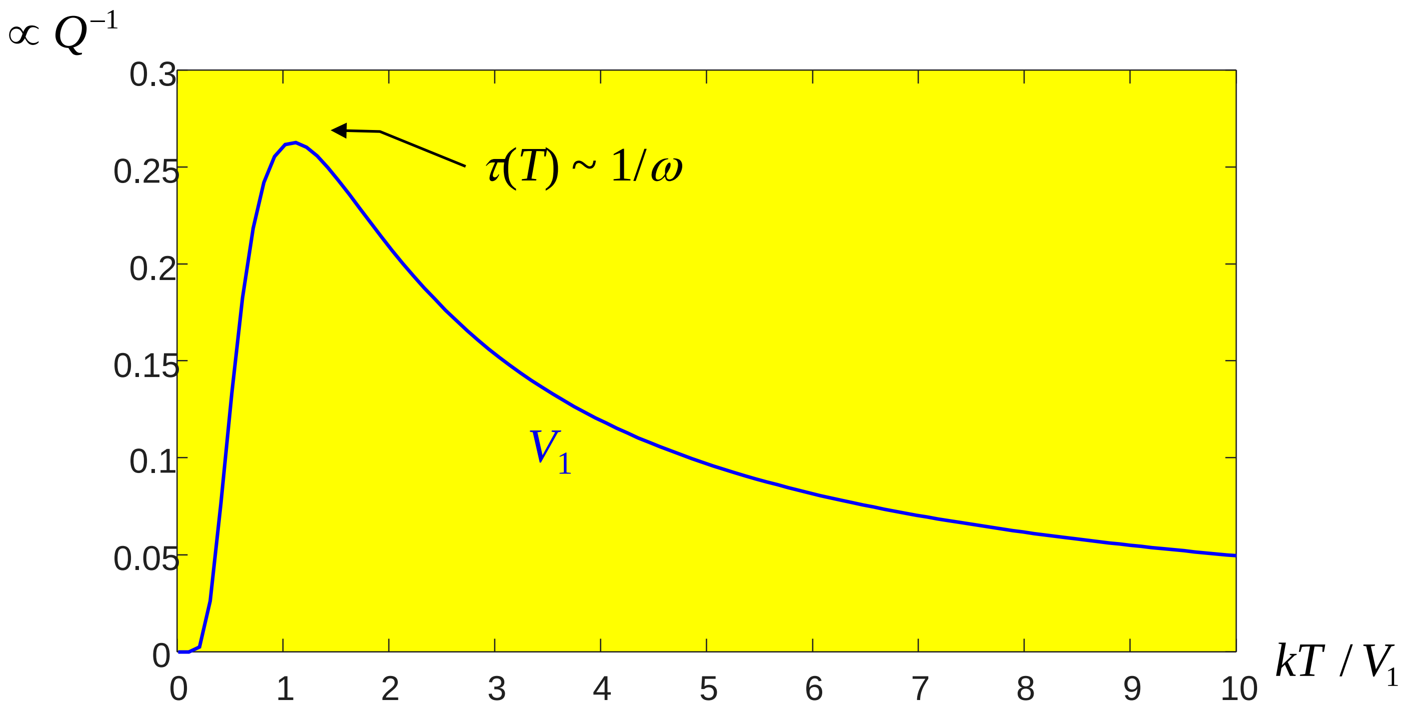
- Above ~5 K, thermally activated rather than quantum tunneling
  - for a single type of TLS:

$$Q^{-1} = N\frac{\gamma^2}{Y\,kT}\frac{\omega\tau}{1+\omega^2\tau^2}\operatorname{sech}^2\left(\frac{\Delta}{kT}\right)$$

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



ω: acoustic frequency



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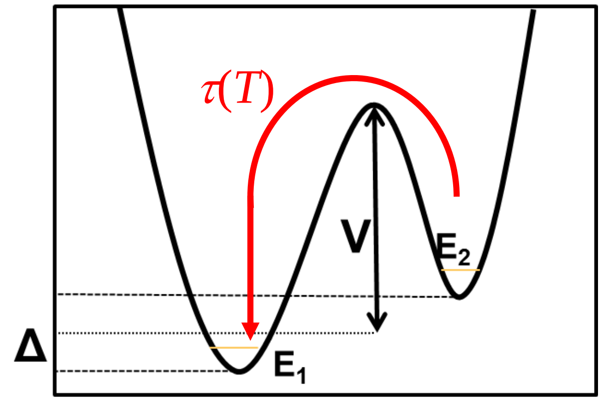
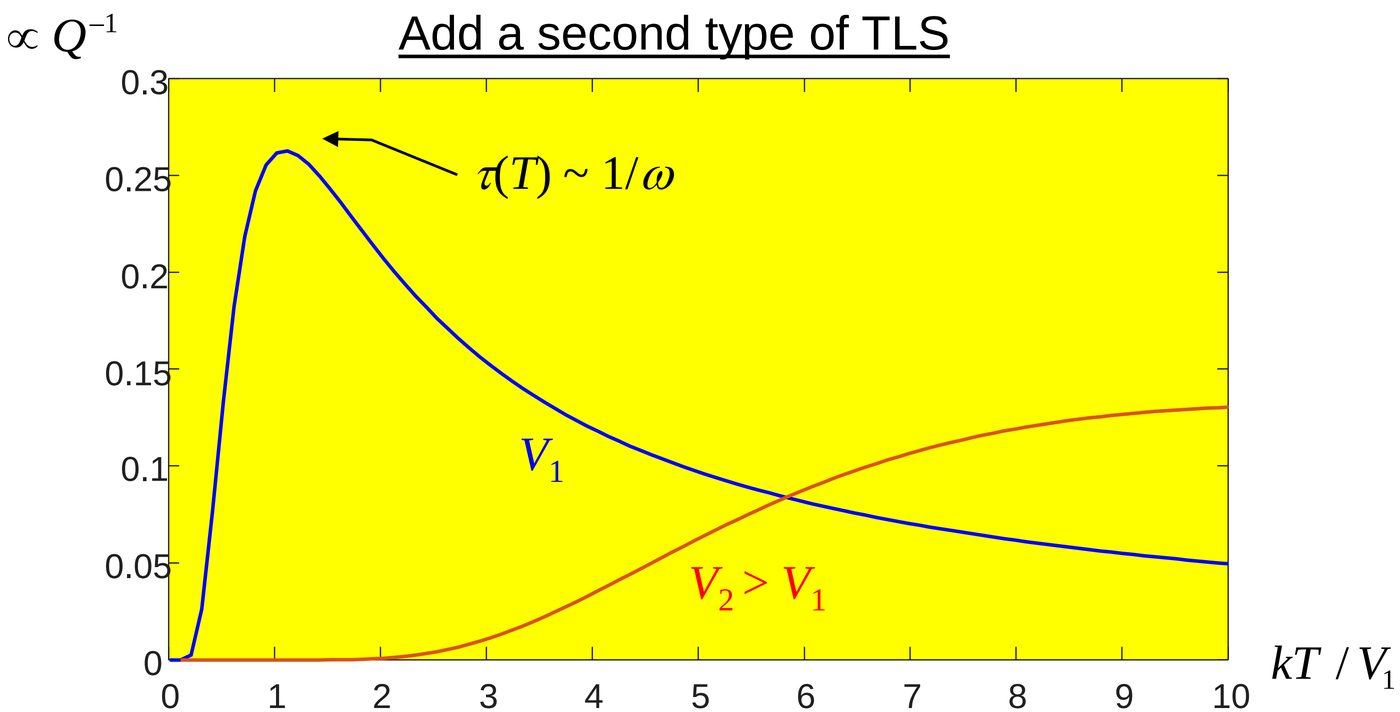


Add a second type of TLS



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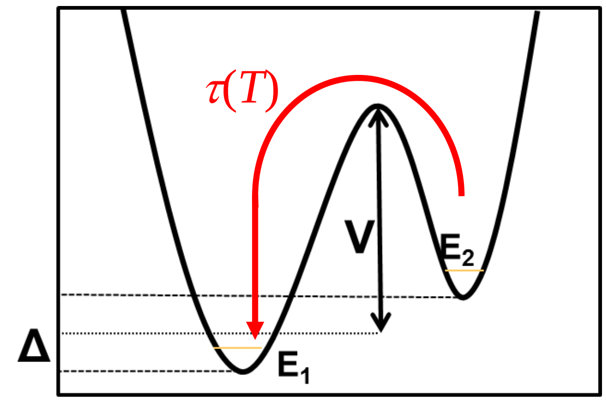

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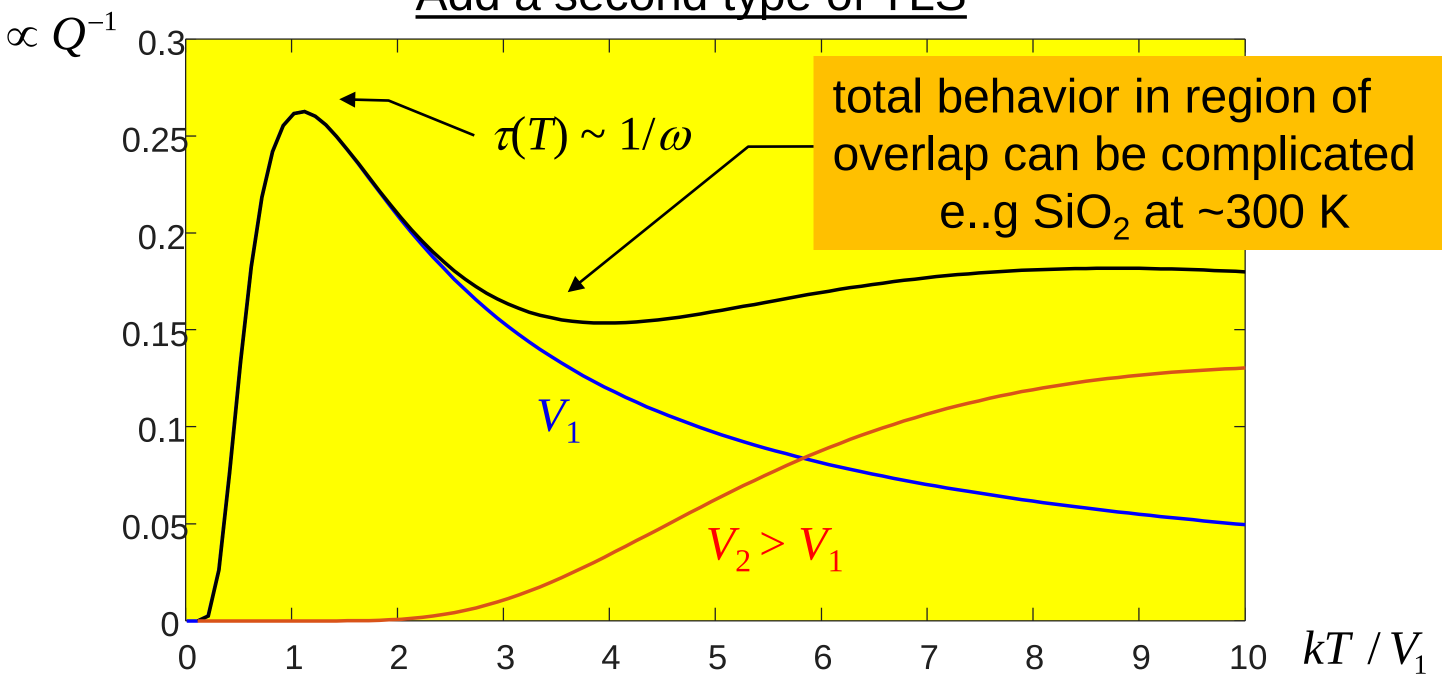


Elastic Dissipation by TLS

- Real materials have distribution of TLS

Gilroy, K. S. and Phillips, W. A., Philos Mag. B, **38,** 735 (1981)

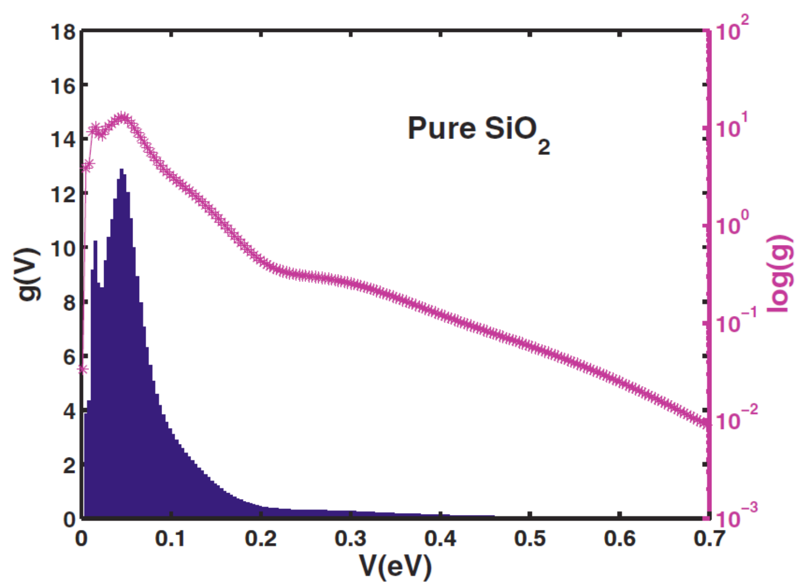
- Dissipation is weighted average of their contributions
  - smears out attenuation function

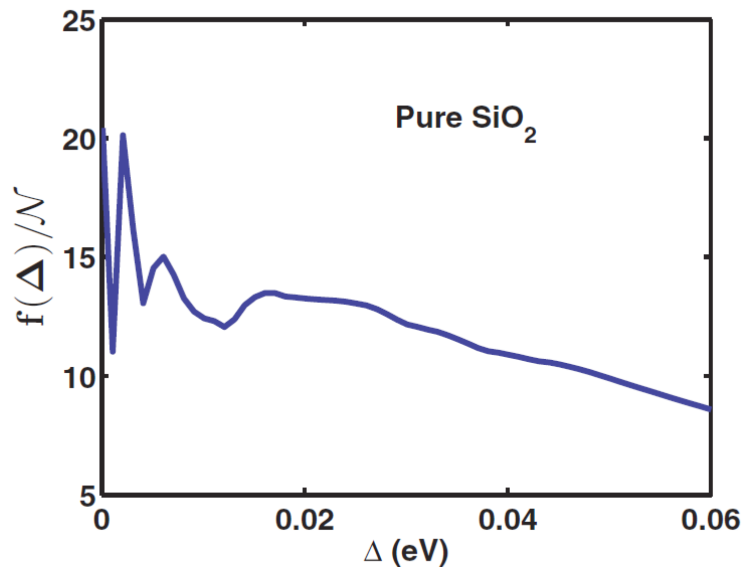
$$Q^{-1} = \frac{\gamma^2}{Y\,kT}\iint \frac{\omega\tau}{1+\omega^2\tau^2}\,\mathrm{sech}^2\left(\frac{\Delta}{kT}\right) g(V)\, f(\Delta)\, dV\, d\Delta$$

barrier height distribution → $g(V)$

asymmetry distribution → $f(\Delta)$

$$\tau(T) = \tau_0\,\mathrm{sech}\left(\frac{\Delta}{2kT}\right) e^{V/kT}$$

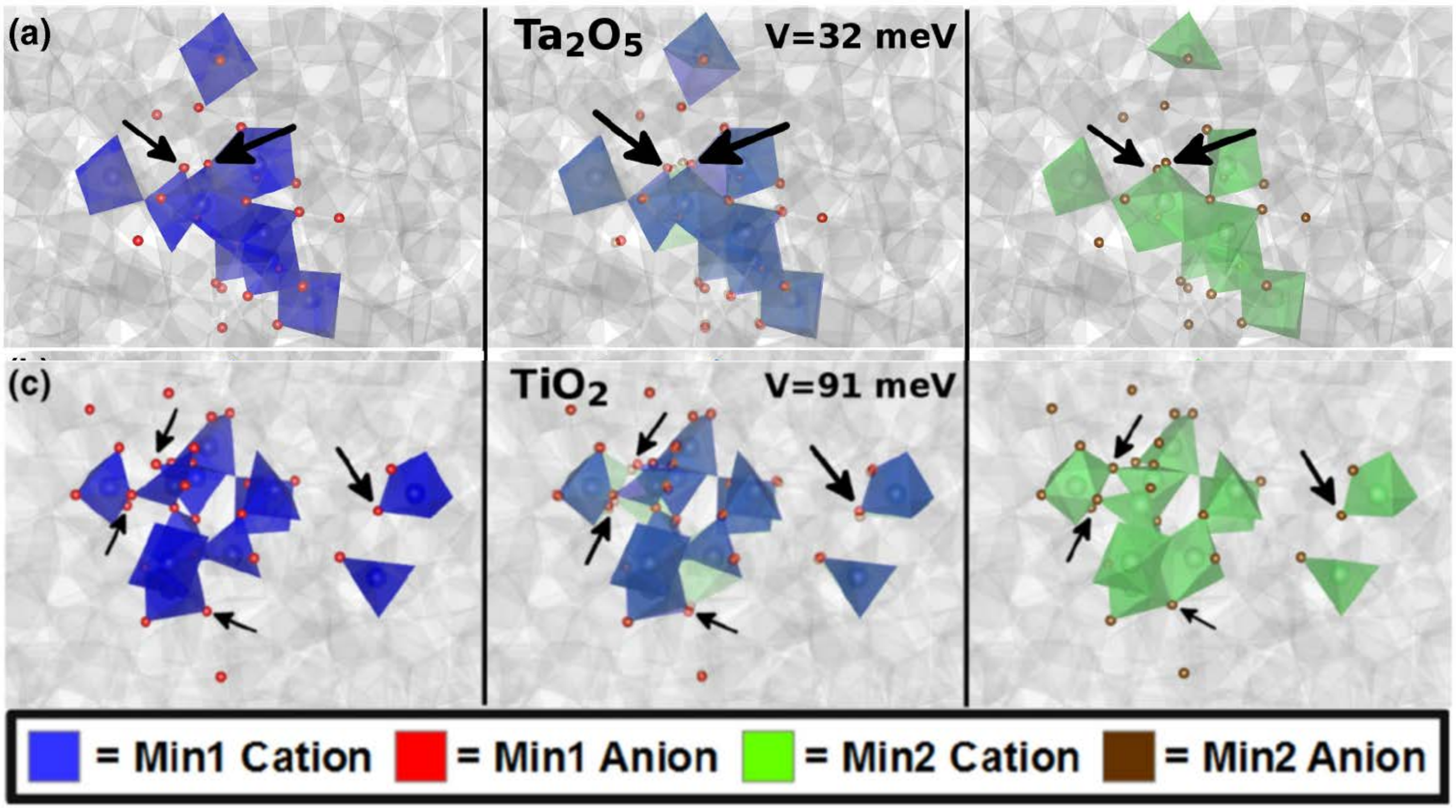




Calculated in R. Hamdan, J.P. Trinastic, and H. P. Cheng, J. Chem.Phys. **141**, 054501 (2014)

Theoretical Guidance: Molecular Dynamics

- Molecular dynamics calculations for amorphous materials
  - provide insight into dissipation mechanisms
  - can suggest promising material combinations
- Some observations: simple bond-flopping inadequate picture
  - TLS involves dozens of atoms in nm-scale configurations

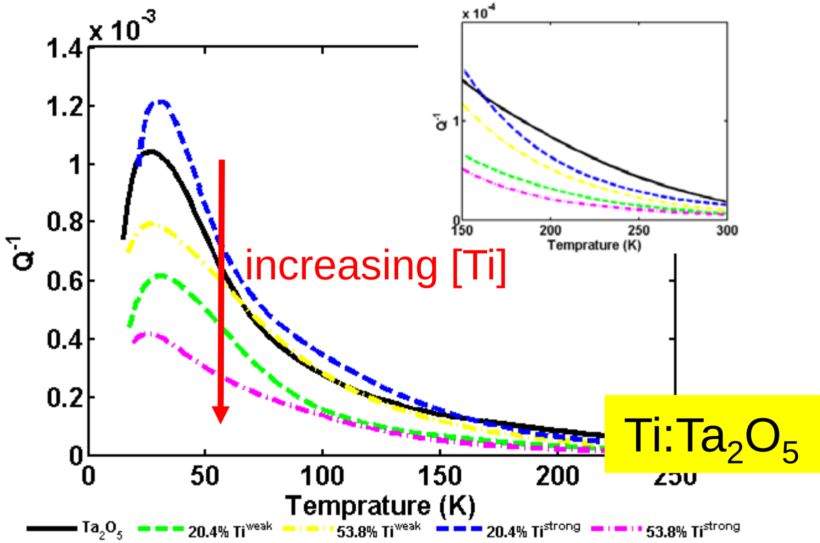


J. Trinastic, R. Hamdan, C. Billman, H. Cheng, *Phys. Rev.* **B93** , 014105 (2016)

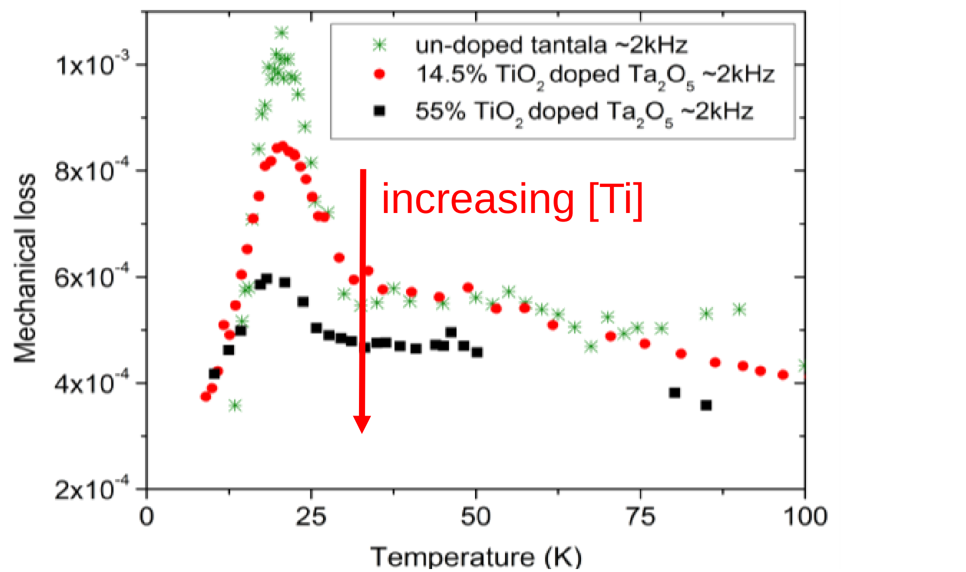
Theoretical Guidance: Molecular Dynamics

- Some observations:
  - some theoretical trends tie up with experiment

    decrease in loss with titania dopoing in tantala



JP Trinastic, *PRB* **93**, 014105 (2016)

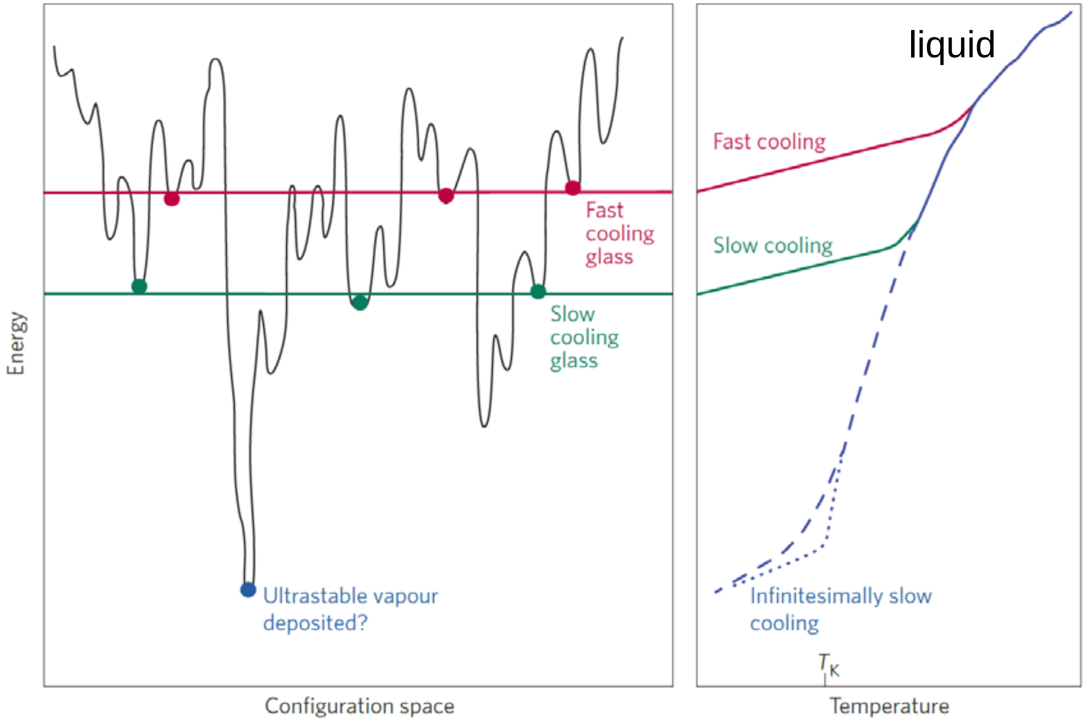


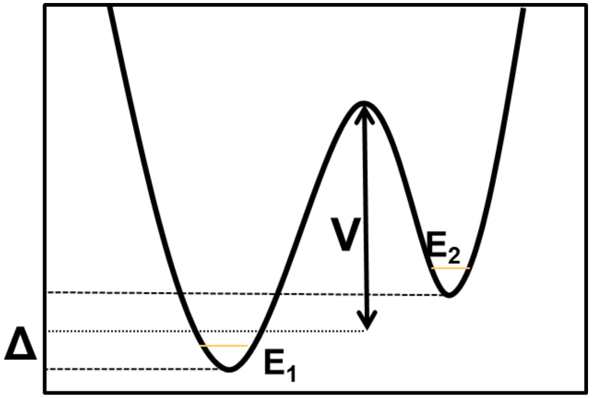
P. Murray et al, U. Glasgow LIGO-G1500874

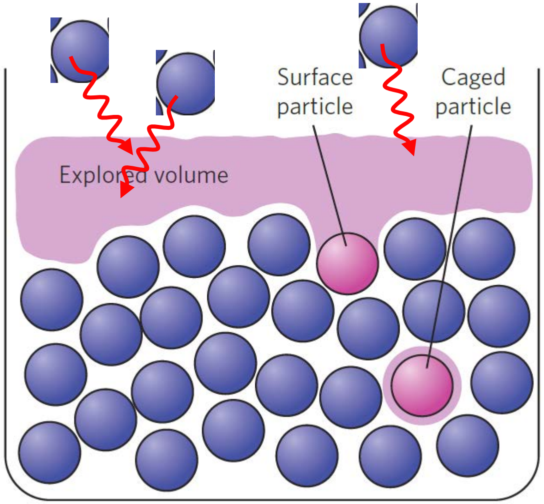
- Correct trends already suggest potentially interesting materials
  - e.g. $ZrO_2:Ta_2O_5$
- Can be extended to model film deposition process
- An issue:
  - agreement worse at higher temperatures than cryogenic

Ultra-stable Glasses

Energy Landscape of Amorphous Materials







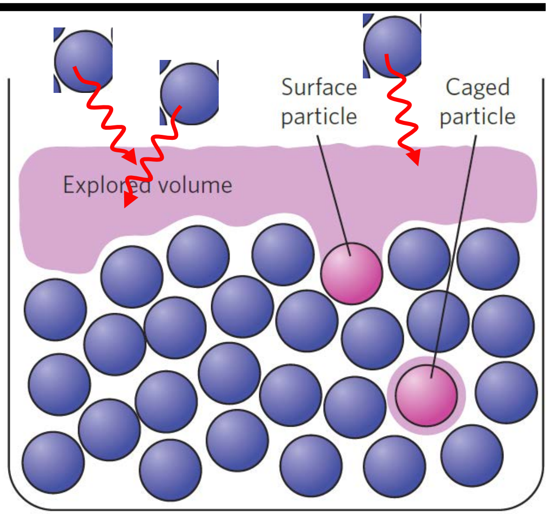
- Slower cooling liquid reaches lower energy states
  - lowest energy states inaccessible from liquid
- Vapor phase deposition accesses lower energies
  - simulations* suggest surface "liquid" layer has orders of magnitude higher mobility than caged particles in solid
  - deposition at high temperature more effective than post-annealing

figures from Parisi, *Nature Mater.* **12,** 94 (2013)

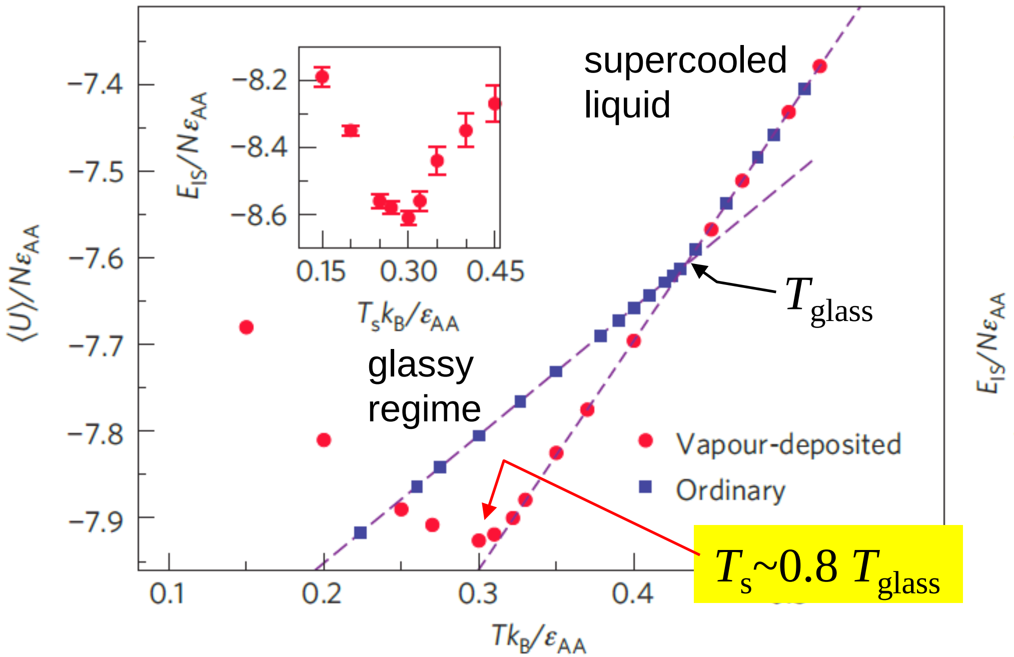
* S. Singh, *Nature Mater.* **12,** 139 (2013)

Simulation of Model System

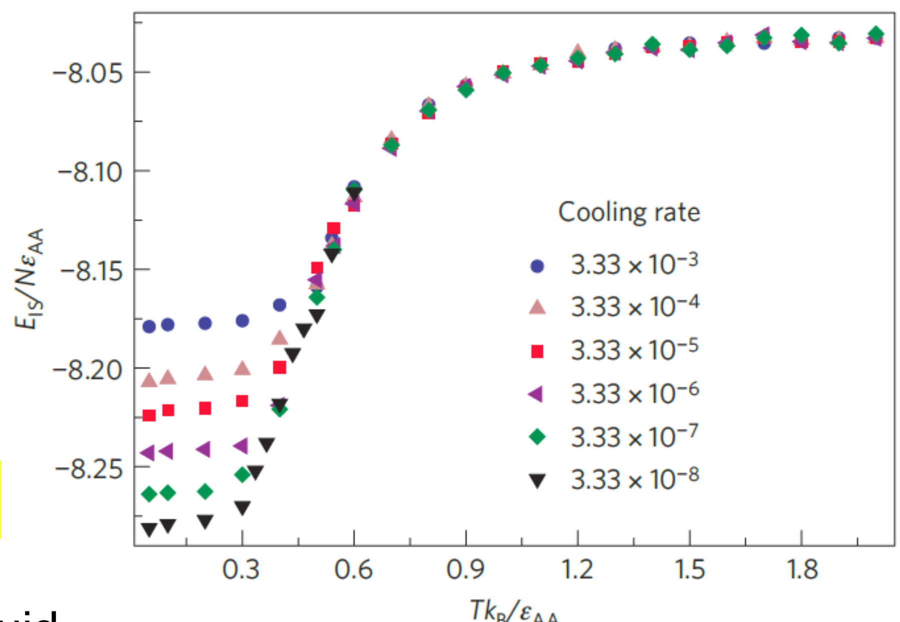
- Add (numerically) Lennard-Jones particles
  - one-by-one onto free surface
  - ~5000 particles
  - explore effect of substrate temperature
  - compare to MD simulation of cooling liquid



<u>liquid vs vapor deposition)</u>



<u>Structure energy (from cooled liquid)</u>



reach more stable glass from vapor than liquid

slow cooling $\Rightarrow$ more stable

S. Singh, *Nature Mater.* **12,** 139 (2013)

Ultra-stable Glasses: amorphous silicon (a-Si)

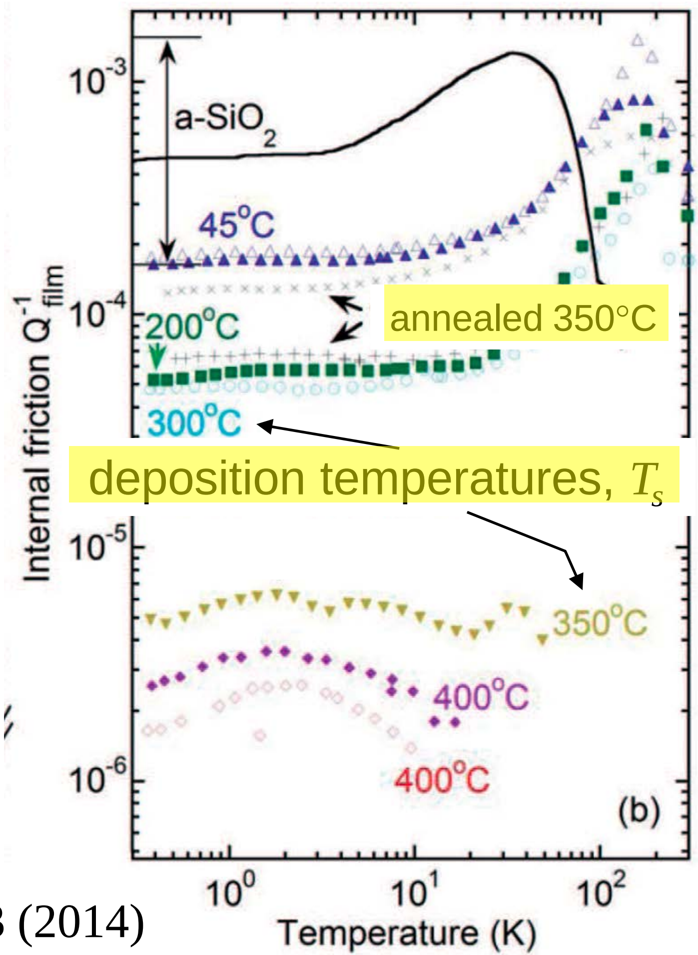
- a-Si experiment: steep improvement for deposition at $T_s \sim$ 400 C: $\phi \sim 10^{-6}$ (!)
  - much lower loss than deposit at 300 C and anneal at 400 C
  - theoretical* $T_{\mathrm{glass}} \sim 900$ K : * C.R. Miranda and A. Antonelli, *J. Chem. Phys.* **120**, 11672 (2004)

    critical $T_s / T_{\mathrm{glass}} \sim 0.75$ vs predicted $T_s \sim 0.8\, T_{glass}$

- Other measures of TLS behave similarly

  specific heat, sound velocity, …
- Similar trends seen in some organics

  T. Perez-Castaneda, *PNAS* **111**, 11275 (2014)



Formation of ultrastable glass favored by:

Deposition at $T_s \sim 0.8\, T_{\mathrm{glass}}$

Low deposition rates

Ion-beam assisted deposition (?)

X. Liu, F. Hellman, et al, *PRL* **113**, 025503 (2014)

Ultra-stable Oxide Glasses for A+?

- a-Si: absorption by dangling bonds an issue at 1 μm
  - explore deposition of ultra-stable oxide glasses for A+

- Experimental work initiated
  - develop vendors for high temperature IBS

    MLD
  - university groups

    UWS: heated substrate, low-rate ECR sputter

    UCB: heated substrate e-beam evaporation

- Open questions: key current topics for experiment and theory
  - unknown glass temperatures for tantala, zirconia, …

    accessible for realistic deposition system?
  - low-rate DIBS an alternative for increased surface mobility?
  - crystallization before formation of ultra-stable glass?

    frustrate with suitable dopant or nanolayers?
  - modelling can help with choices here

Need Alternatives if High-Temp Deposition Fails

- Higher annealing temperatures for oxide glasses
  - push toward more uniform glass, even if not ultra-stable

- Frustrate crystallization *with suitable dopant*
  - suitable stabilizing dopant, e.g. Zr:Ta_2O_5

    Zirconia(34%)-Tantala: $T_{\mathrm{anneal}} = 800$ C, $n \approx 2.1$-2.2 , Y = 134 GPa

    $\phi = 1.4 \times 10^{-4}$ at 300 K [S. Penn, preliminary], potentially useful

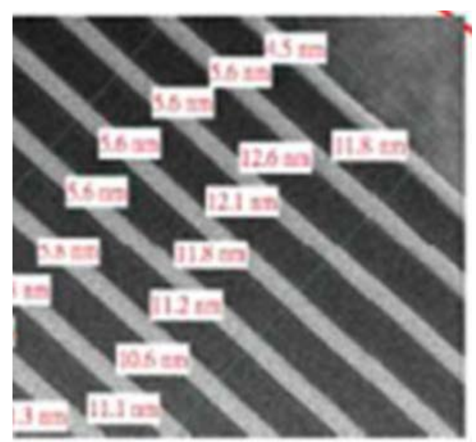
- Frustrate crystallization *geometrically*: “nanolayers” [S. Chao, LIGO-G1300921]

  [Chao, Pinto, DeSalvo]
  - intersperse thin stable (SiO_2) layers in high index material
  - TiO_2/SiO_2 nanolayers: 19 sublayers

    $T_{\mathrm{anneal}} = 300$ C, crystallization suppressed

    $\phi \approx 10^{-4}$
  - volume/interface scatter an issue?
  - new Sannio coating facility

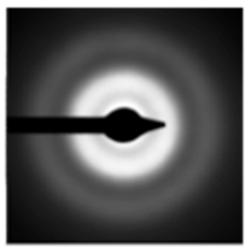
    move beyond few nm layer

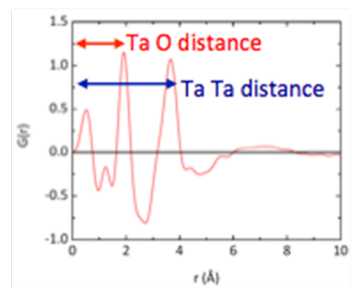


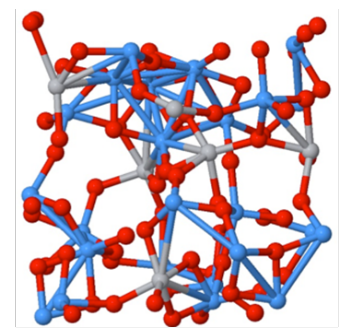
Atomic Structure: Short Range Order

- Characterization of structure of amorphous materials more difficult than crystalline
  - several applicable techniques:

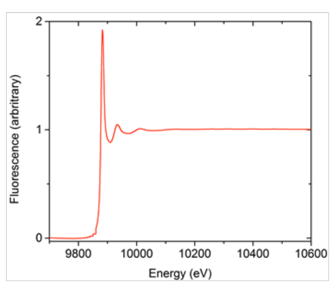
- Short-range order (<1 nm):
  - TEM, NMR, XAFS, Raman
    - Pair Distribution Function (PDF), G(r), electron or X-ray diffraction

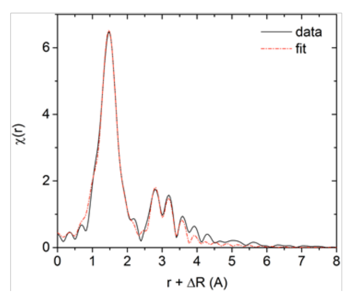






    - Extended X-ray Absorption Fine Structure (EXAFS),
      - Ta L_{III} edge

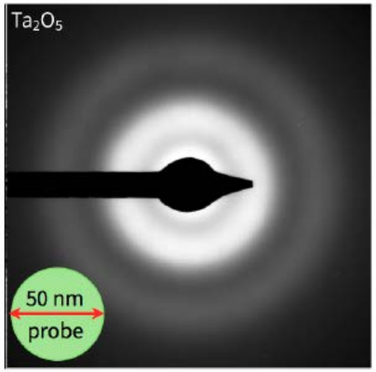


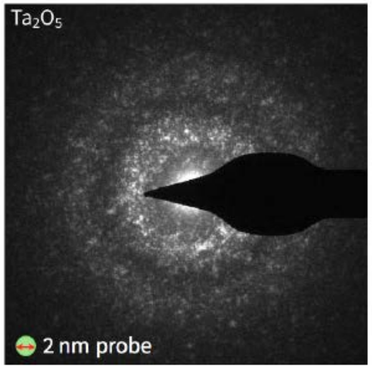


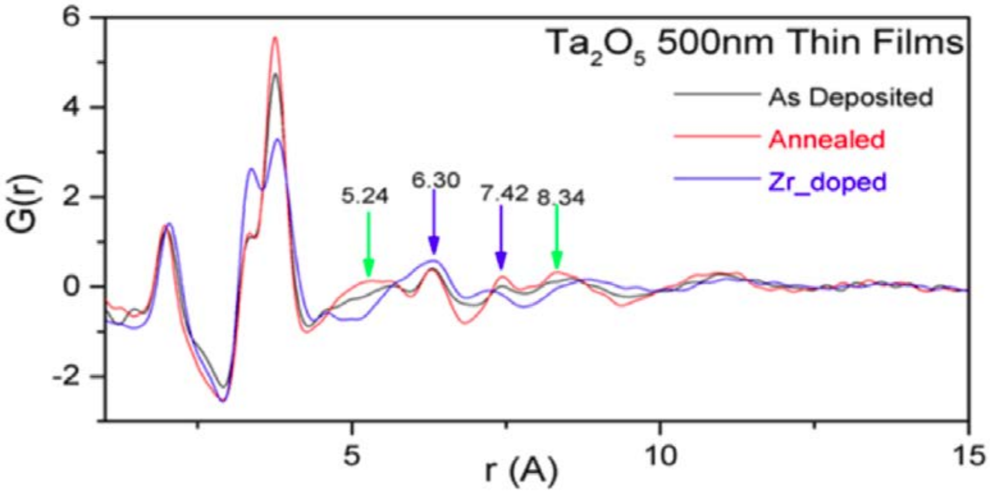
Atomic Structure: Medium Range Order

- Characterization of structure of amorphous materials more difficult than crystalline
  - several applicable techniques:

- Medium-range order (0.5 – 5 nm)
  - particularly relevant to extended TLS
  - fluctuation electron microscopy
  - GI-XRPDF



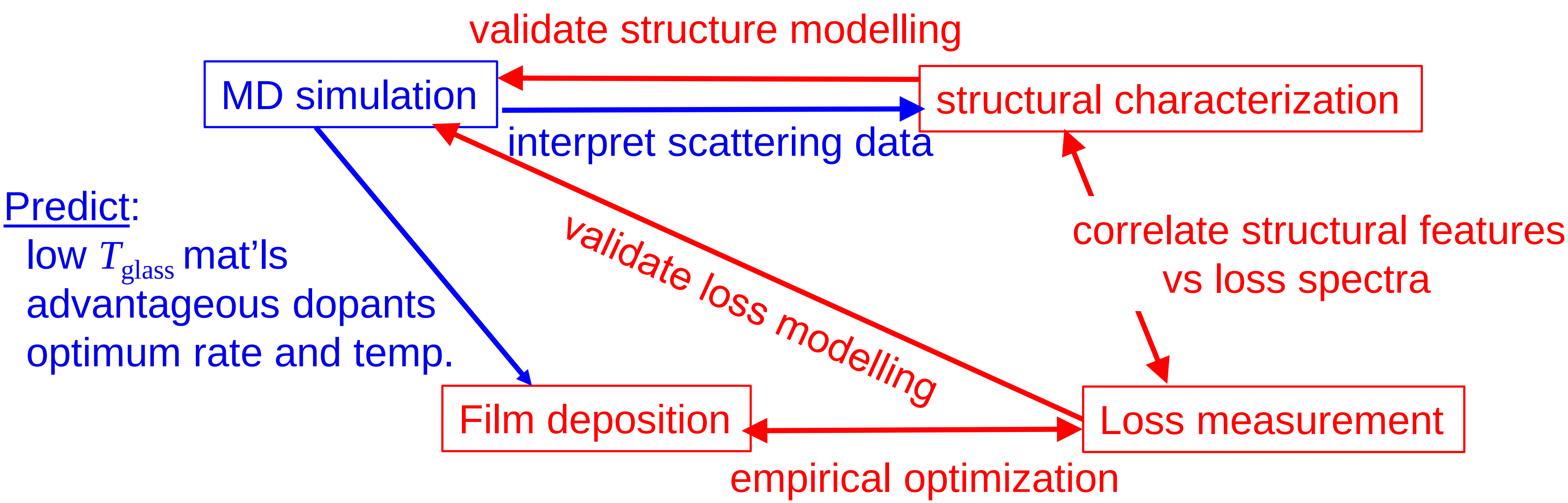




How to Use Structural Characterization

- Some observations:
  1. structural changes with annealing and doping are subtle
  2. difficult to unambiguously invert from data to structure
  3. forward calculations advantageous vs inverse for structural data

Experiment and theory reaching maturity to usefully interact



Summarizing Current Directions in A+ Coating Research

- Ultra-stable oxide glasses: experiments beginning
  - high temperature deposition
  - ion beam sputtering/ion assisted
  - slow deposition rates

- Other experimental approaches to synthesize lower loss coatings:
  - nanolayer stabilization
  - dopant-stabilized high-temperature annealing
  - multi-material coatings

- Atomic structure modeling/characterization
  - experiment and theory reaching maturity to usefully interact
  - tie-up loss and structure modeling with measurements
  - explore theoretically advantageous material/dopant combinations

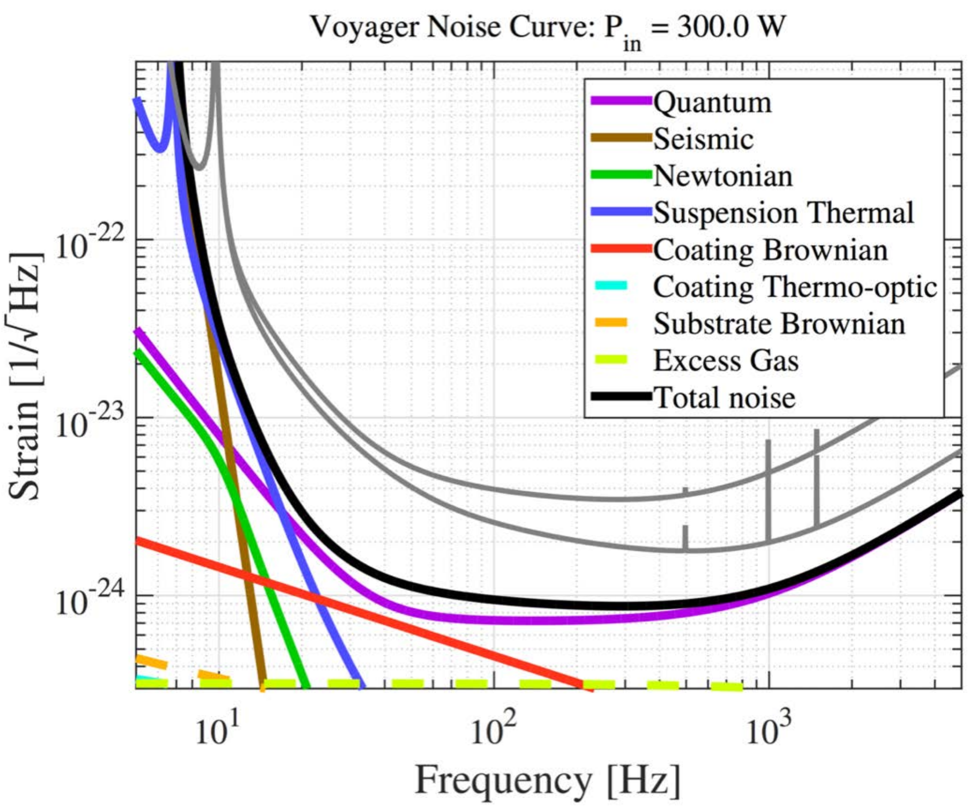
Voyager: Cryogenic LIGO (2025?)

Mirrors:
160 kg Silicon substrate
123 K

Laser:
λ = 1.5 – 2.x μm
P_{stored} = 2 MW

8 dB squeezing

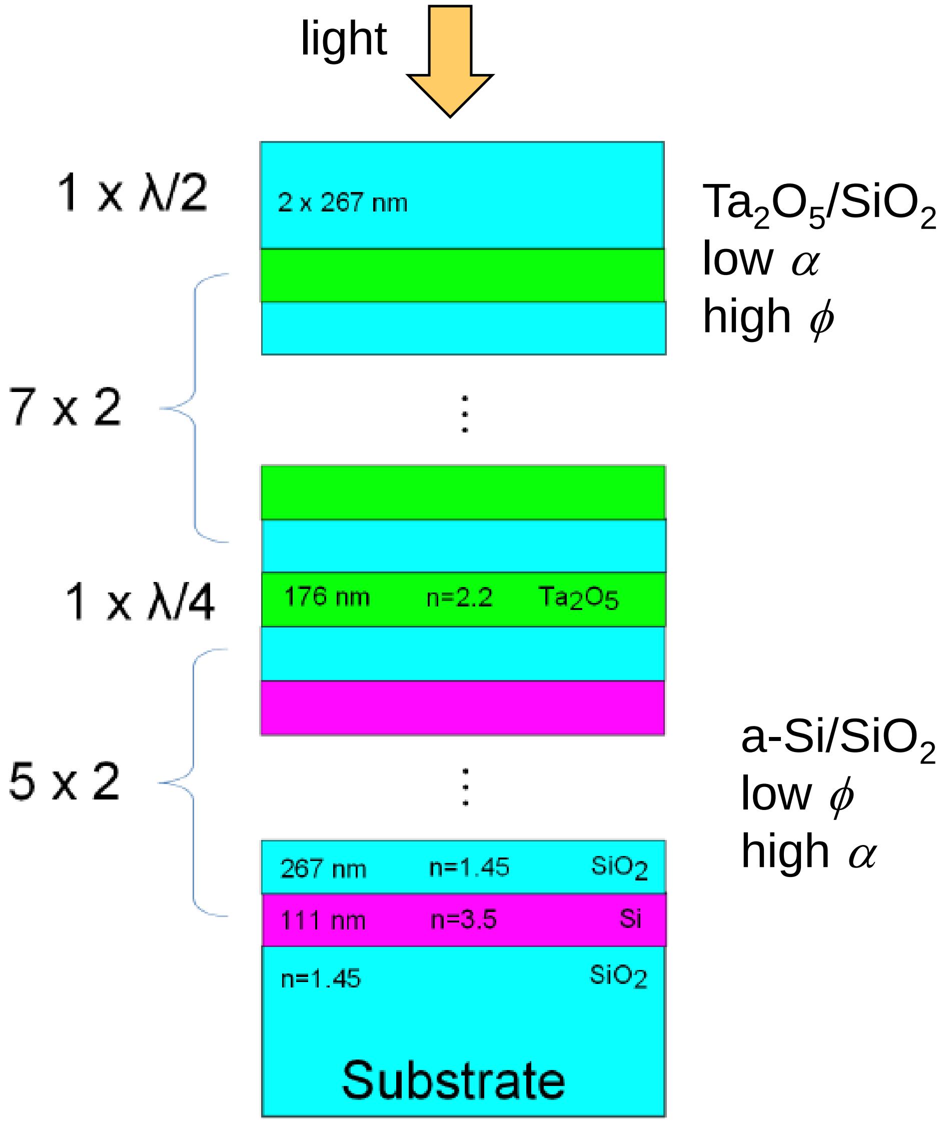
Coating Thermal Noise:
Additional 3-5x reduction
ϕ ~ 2–4 x 10^{-5}



LIGO Instrument Science White Paper 2015
https://dcc.ligo.org/DocDB/0120/T1500290/002/T1500290.pdf

$\lambda \sim 1.5 - 2$ μm Facilitates Use of a-Si

- Absorption from dangling bonds too high at 1 μm
  - ~10x worse at 1 vs 1.5 μm
  - reduced by high T_s
    but ~2x, not 10^3x
- Multi-material coatings could mitigate absorption
- Recent IBS at UWS promising
  - hot substrate, low-rate ECR
    20 ppm @ 1.5 μm with a-Si/SiO_2
    S. Reid
    [https://dcc.ligo.org/LIGOG16012]00]
  - IBS in H^+ containing plasma
    promising initial results
    D. Gibson [ThC.2 OIC 2016]



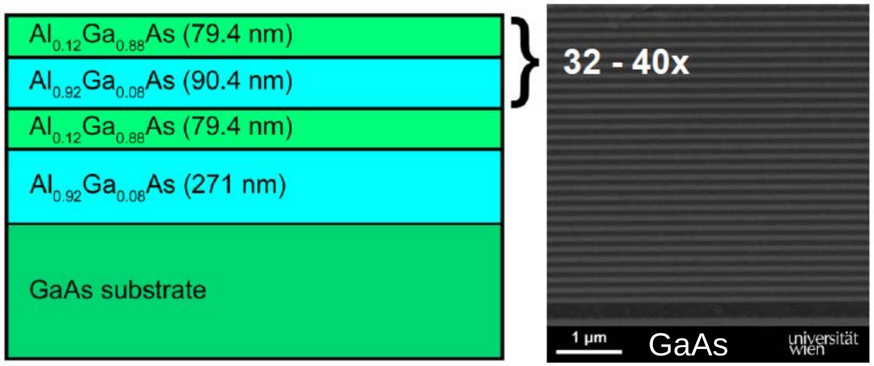
J. Steinlechner, et al , *Phys. Rev. D* **91** 042001 (2015)
W. Yam et al, *Phys. Rev. D* **91**, 042002 (2015)

Crystalline Coatings

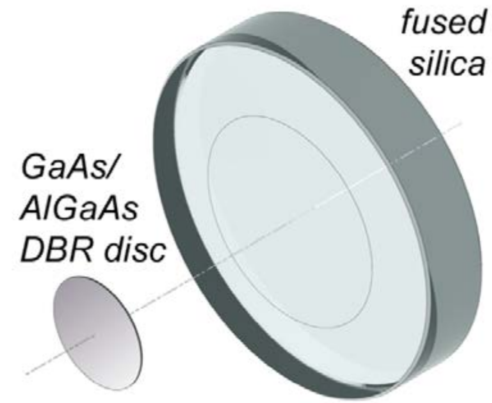
- GaAs/AlGaAs epitaxy on GaAs, transferred to mirror substrate

$\phi \sim 2 \times 10^{-5}$, $\alpha < 1$ ppm

G. Cole, LIGO-G1401152



G. Cole, Crystalline Mirror Solutions

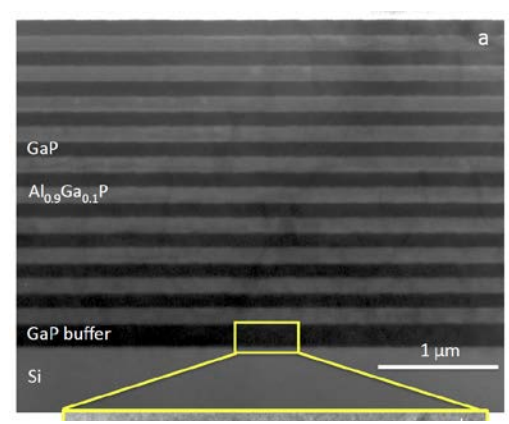


- GaP/AlGaP epitaxy on Si mirror substrate

A. Lin, SU: $\phi < 1 \times 10^{-4}$, $\alpha = ??$

new AlGaP MBE, S. Reid, UWS

A. Lin, SU, LIGO-G1200135



Key challenges for any crystalline coating:
scatter loss not yet measured over large areas
MBE tool maintaining nm uniformity over 34 cm: $$$

AlGaAs: GaAs substrates, bonding over large area
AlGaP: investigation of absorption mechanisms

Summary

- A+ [1.06 μm, 300 K, 2019(?)]
  - ultra-stable oxide glasses

    hot substrates, ion beam assist, low rates
  - stabilized annealing

    suppressed crystallization with dopants or nanolayers
  - atomic structure modeling and experiment

    at stage where can inform each other and synthesis choices
- Voyager [1.5 – 2.x μm, 120 K, 2025(?)]
  - ultra-stable glasses

    oxide, a-Si
  - crystalline coatings
- Explorer ?