Coatings -- roadmap to readiness

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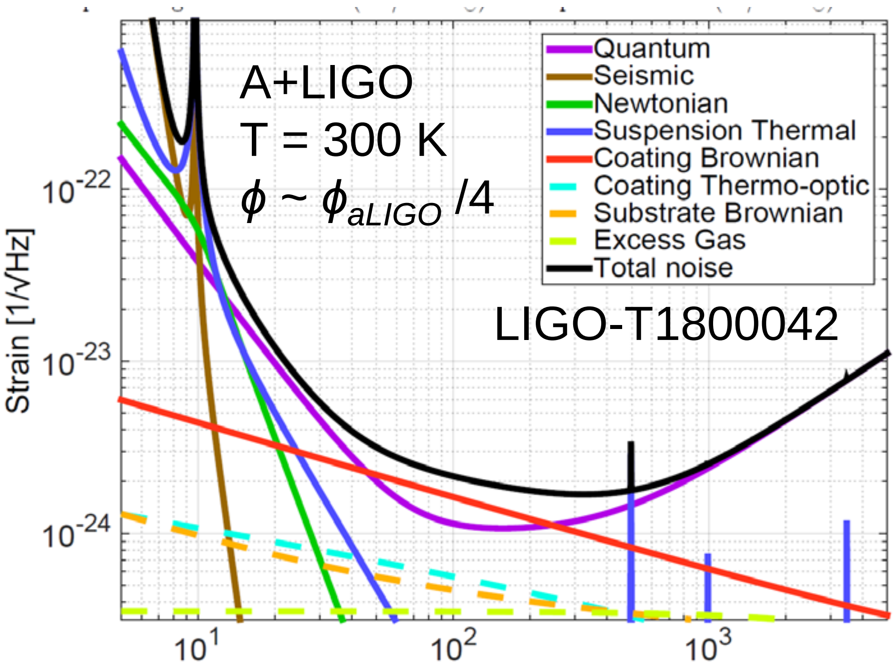
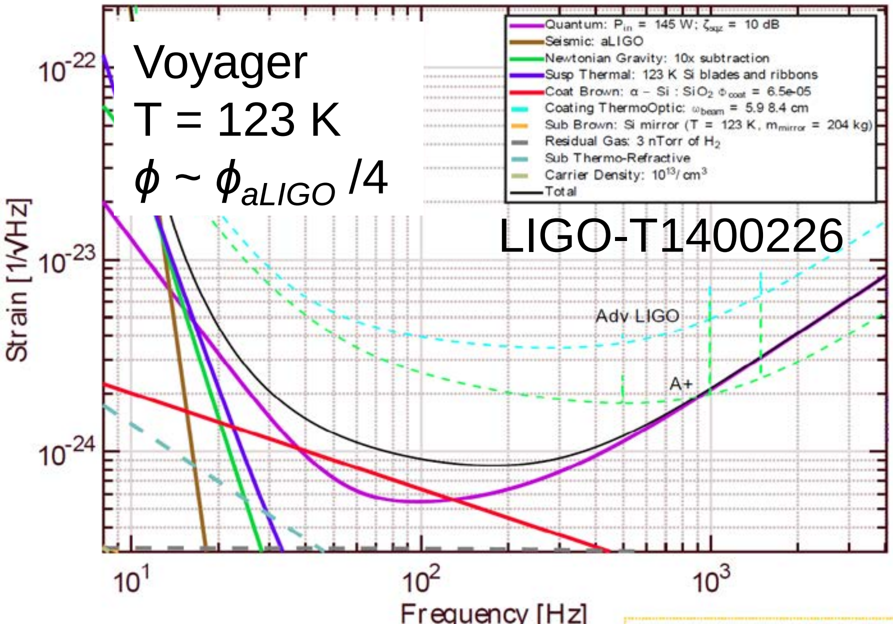
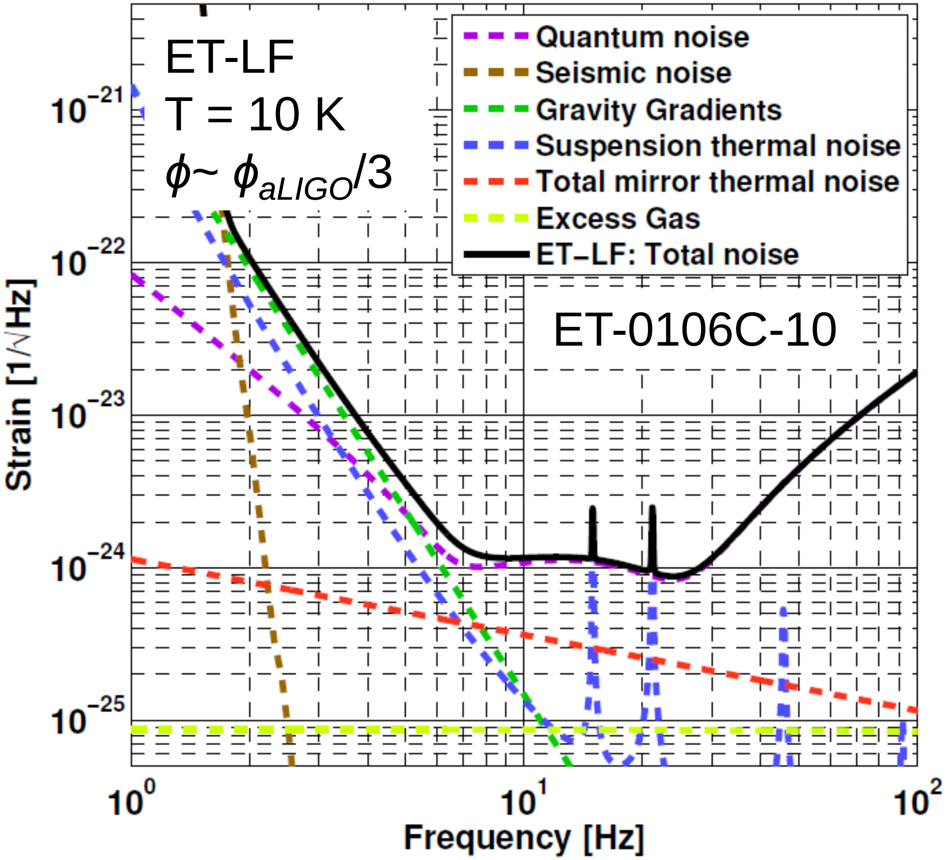
31 August, 2018

Why are coatings an issue?

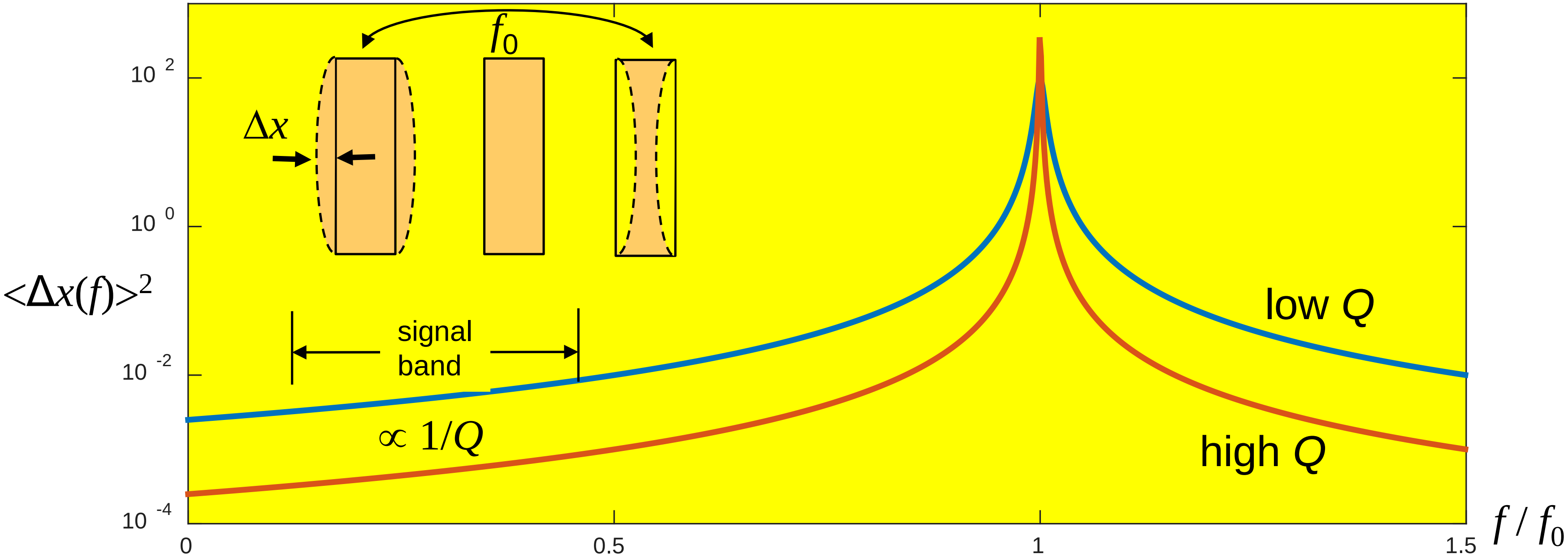






- Thermal noise limits mid-band sensitivity
- Coatings dominate thermal noise

Thermal Noise in IF Mirrors



- Oversimple: kT of energy per mechanical mode, viscous damping
  - moves front of mirror w.r.t. center of mass

- For coating dominated noise and structural damping:

coating elastic loss

$\phi \equiv \mathrm{Im}Y \,/\, \mathrm{Re}Y$

coating thickness

cryogenic

$$\left\langle \Delta x(f,T)^2 \right\rangle \approx \frac{2k_B T}{\pi^2 f}\frac{d}{w^2 Y}\phi(f)$$

beam radius

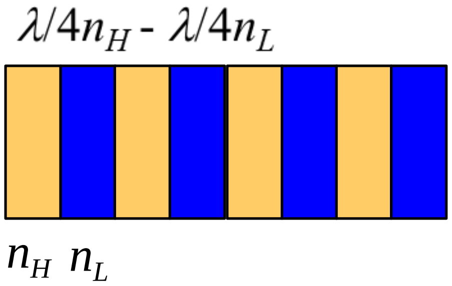
aLIGO:

$$\boxed{\begin{aligned}\phi_{\mathrm{TiO_2:Ta_2O_5}} &= 2.3\times10^{-4}\\ \phi_{\mathrm{SiO_2}} &= 4\times10^{-5}\end{aligned}}$$

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

Basic Coating Concepts

$$\left\langle \Delta x(f,T)^2 \right\rangle \approx \frac{2k_BT}{\pi^2 f}\frac{d}{w^2 Y}\phi(f)$$



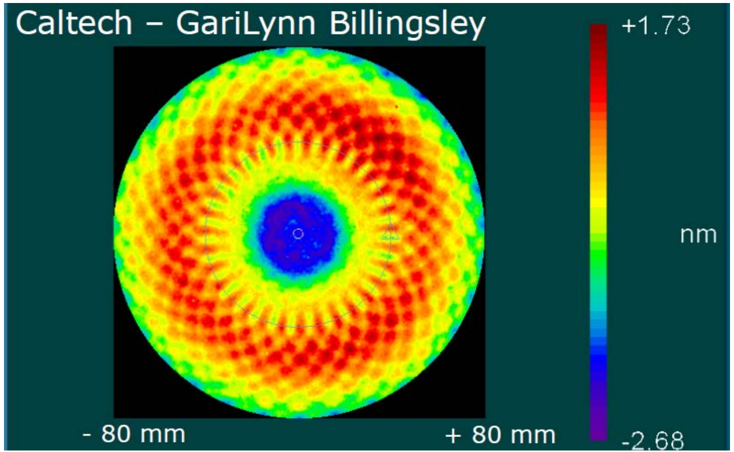
- Dielectric mirror
  - alternating high/low index ¼ wavelength-thick layers
  - large index contrast ⇒ fewer required layers: $d \sim 1/(n_H - n_L)$

$$F.O.M.(roughly) \sim \frac{\phi}{n_H - n_L}$$

- Key optical properties
  - absorption, scatter – ppm’s
  - industry standard: ion-beam sputtering

    R.T. deposition followed by 300 C – 500 C annealing
  - scaling to >30 cm nontrivial

    with ~1 nm RMS figure: LMA, Lyon



Typical Requirements

	T (K)	λ (µm)	$\phi / \phi_{a\text{-}LIGO}$	HR abs.
A+	300	1	1/4	0.5 ppm
Voyager	123	~2	1/4	2 ppm
ET-LF	10 – 20?	1.5?	1/3	~1-5 ppm

- Explorer:
  - A+ or Voyager coating solution can be applied

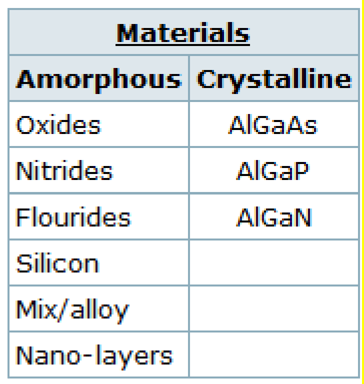
    though larger optics and higher power

- No magic bullet solution meets all requirements
  - brief view of physics to motivate approaches

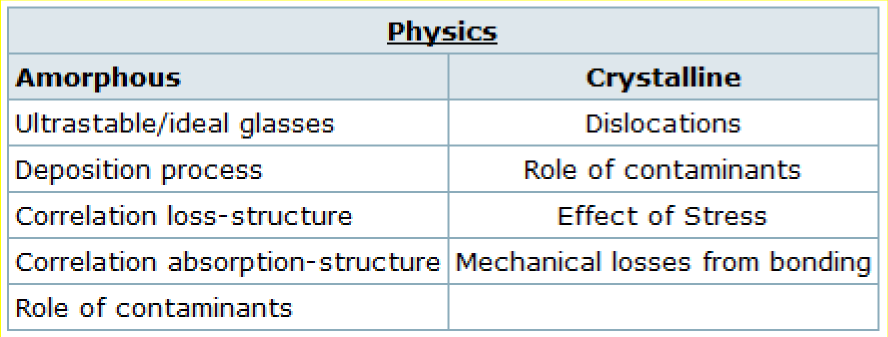
- Present examples of representative approaches

The Context of Coatings Development

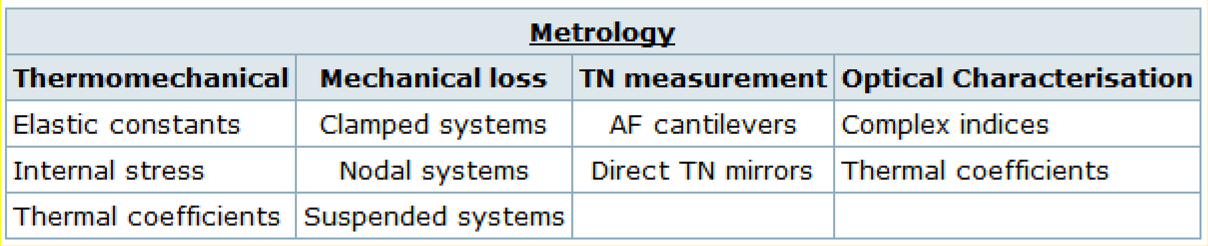
- Materials



Materials	
Amorphous	**Crystalline**
Oxides	AlGaAs
Nitrides	AlGaP
Flourides	AlGaN
Silicon	
Mix/alloy	
Nano-layers	

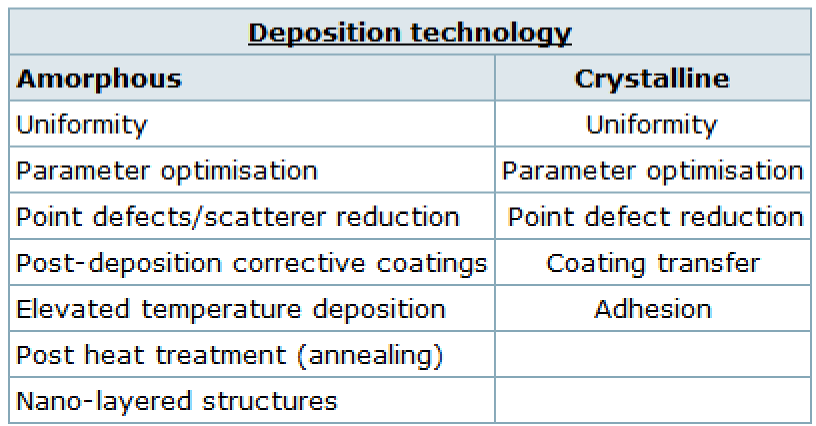


Physics	
Amorphous	**Crystalline**
Ultrastable/ideal glasses	Dislocations
Deposition process	Role of contaminants
Correlation loss-structure	Effect of Stress
Correlation absorption-structure	Mechanical losses from bonding
Role of contaminants	



Metrology			
Thermomechanical	**Mechanical loss**	**TN measurement**	**Optical Characterisation**
Elastic constants	Clamped systems	AF cantilevers	Complex indices
Internal stress	Nodal systems	Direct TN mirrors	Thermal coefficients
Thermal coefficients	Suspended systems		

- Deposition and related metrology



Deposition technology	
Amorphous	**Crystalline**
Uniformity	Uniformity
Parameter optimisation	Parameter optimisation
Point defects/scatterer reduction	Point defect reduction
Post-deposition corrective coatings	Coating transfer
Elevated temperature deposition	Adhesion
Post heat treatment (annealing)	
Nano-layered structures	

G. Cagnoli

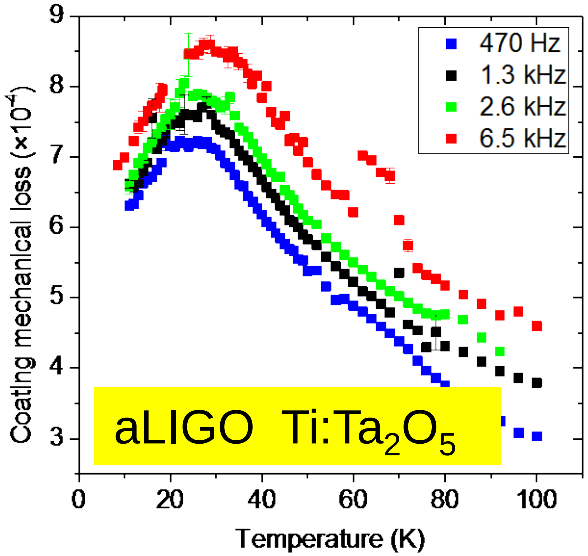
General Observations About Coating Elastic Loss

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

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

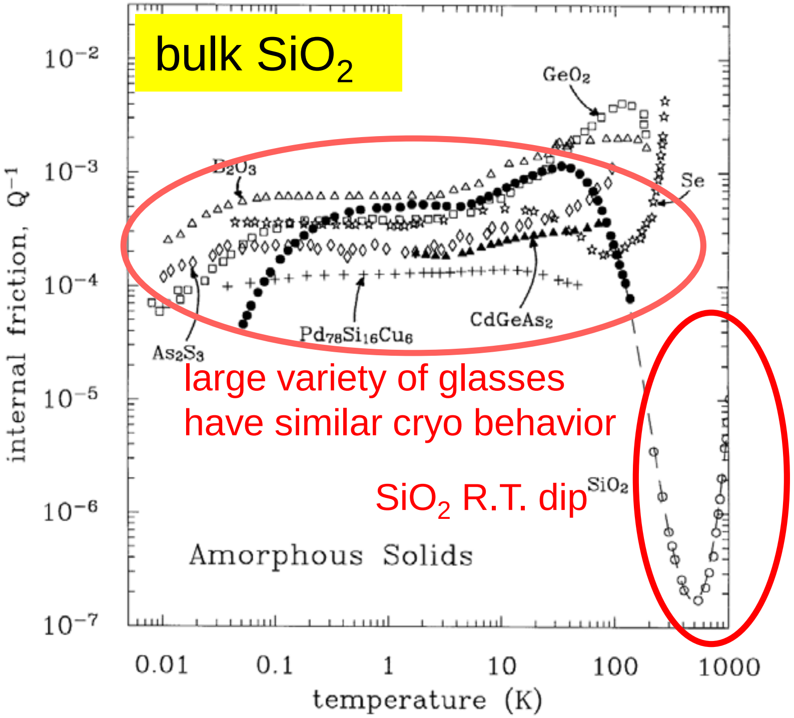
  - current values: Ti:tantala ~5x lossier than silica

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



aLIGO Ti:Ta$_2$O$_5$

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



bulk SiO$_2$

large variety of glasses have similar cryo behavior

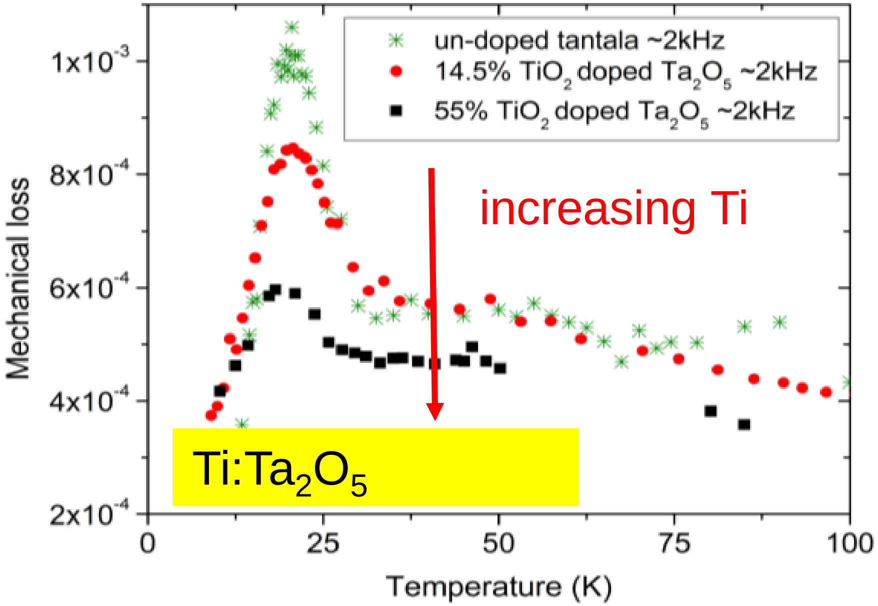
SiO$_2$ R.T. dip

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

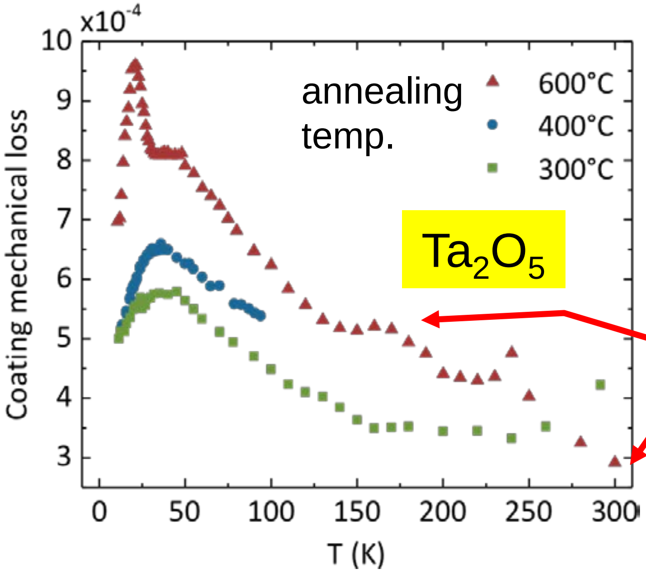


increasing Ti

$Ti:Ta_2O_5$

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

- Annealing modifies loss spectra



Ta_2O_5

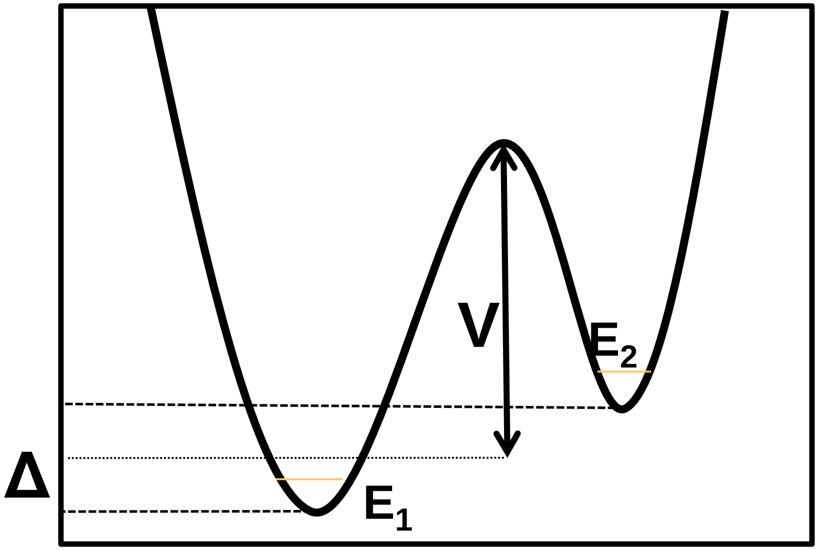
[I W Martin et al, Class. Quant. Grav. 27 225020, 2010]

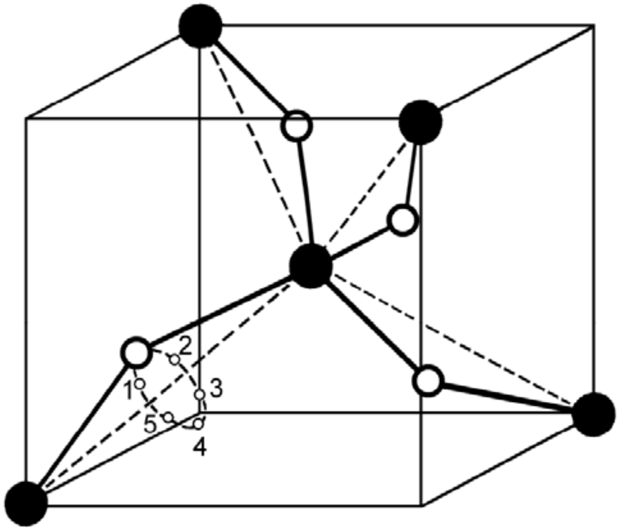
annealing modifies behavior
can improve loss at some temperatures
while worsening it at others

annealing temperature limited by crystallization
suppressing crystallization important

Low-frequency losses in amorphous dielectrics

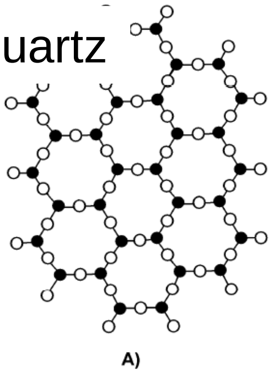
- Conventionally associated with low energy excitations (LEEs)
  - conceptualized as two-level systems (TLS)

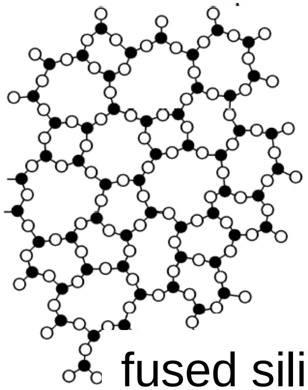




Oversimple picture: bond flopping

crystal quartz





fused silica

(●= Si, ○ = O).

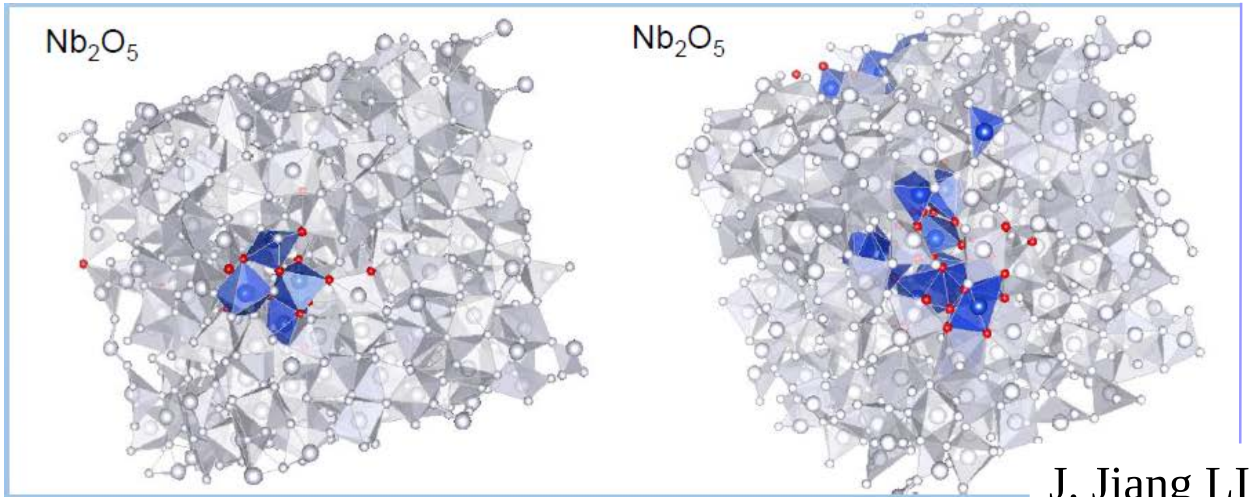
Distribution of TLS in silica due to disordered structure

figures from B.S. Lunin monograph

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 fails
  - TLS involves dozens of atoms in nm-scale configurations

    “medium-range” order important



J. Jiang LIGO G1800533

Atoms involved in a low energy barrier (24.142 meV) TLS

Atoms involved in a high energy barrier (481.442 meV) TLS

cause cryogenic losses

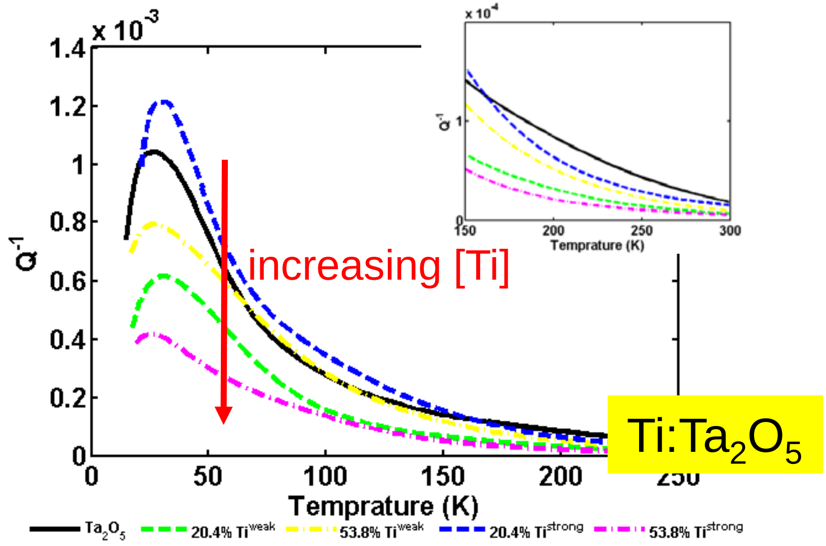
cause 300 K losses

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

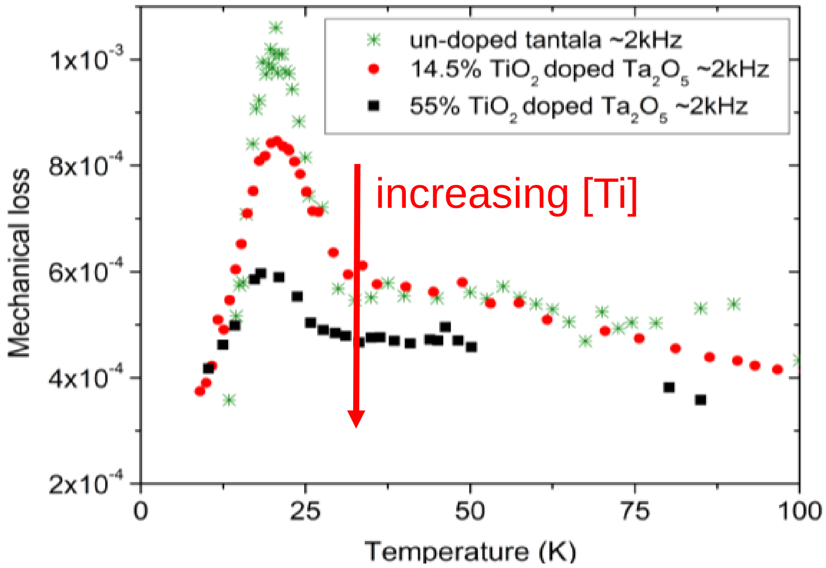
Theoretical Guidance: Molecular Dynamics

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

    decrease in loss with titania dopoing in tantala



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



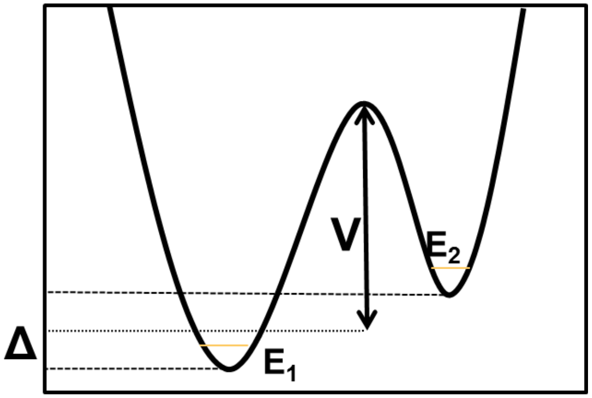
P. Murray et al, U. Glasgow LIGO-G1500874

- Correct trends already suggest potentially interesting materials
  - e.g. $ZrO_2:Ta_2O_5$ (more later)

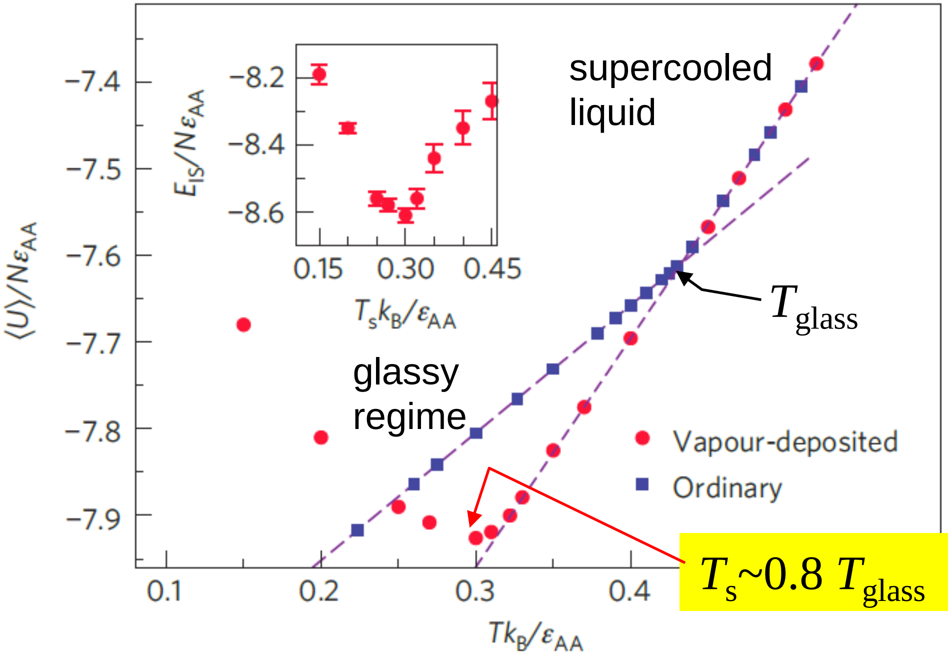
- Agreement best at cryogenic temperatures

    larger models being implemented to address 300 K range

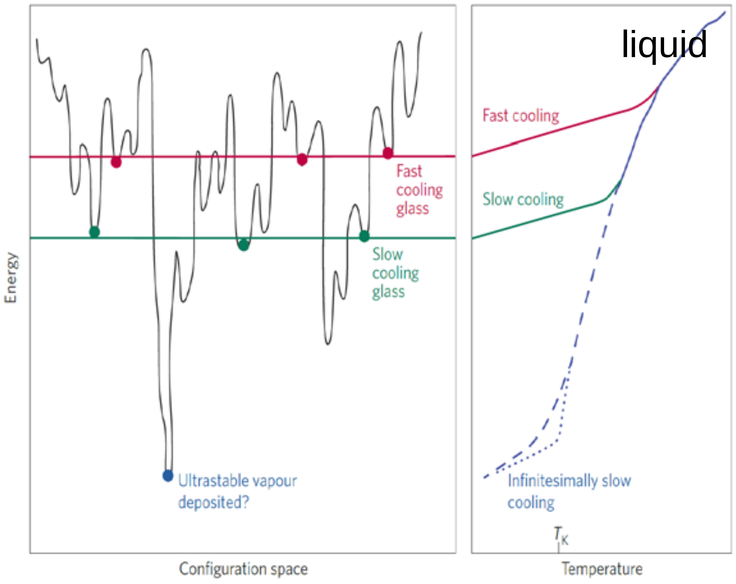
Ultrastable Glass: Toy Model

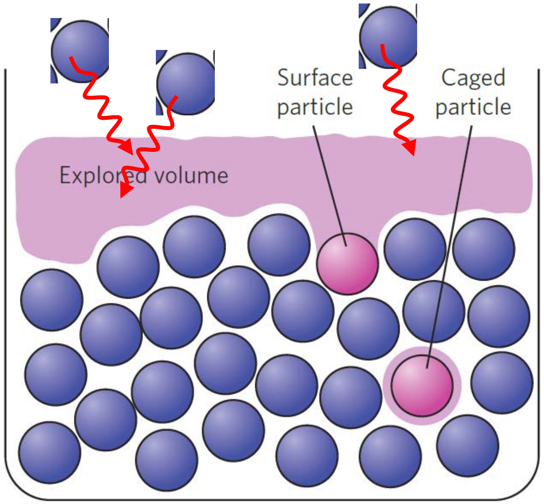


<u>liquid vs vapor deposition)</u>



reach more stable glass from vapor than liquid





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

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

- First example of inorganic ultra-stable glass
  - potential for Voyager mirror coating

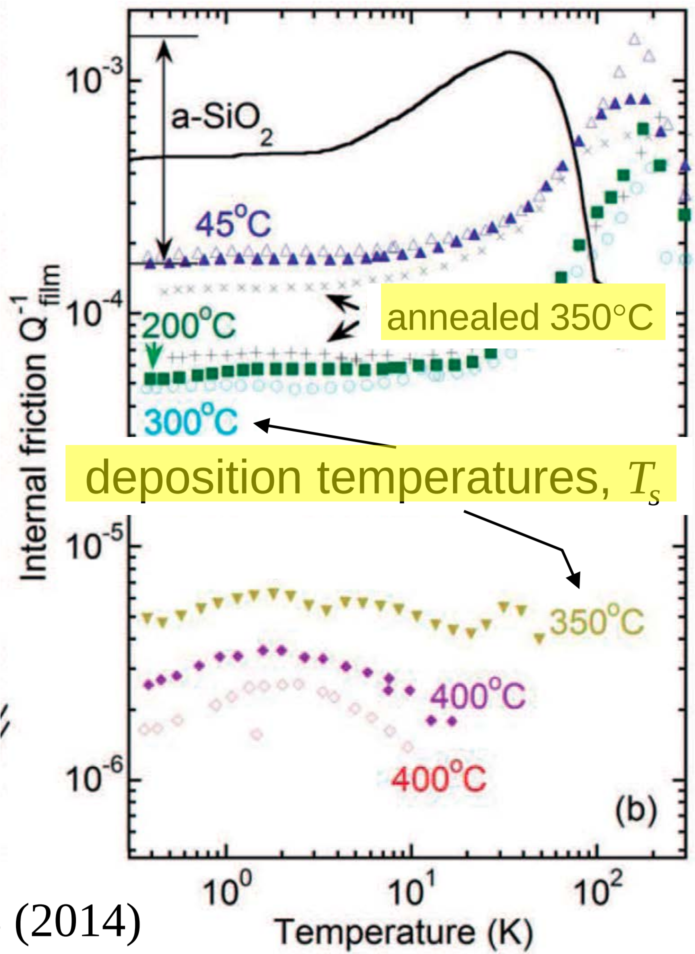
Formation of ultrastable glass favored by:

Deposition at $T_s \sim 0.8\ T_{\text{glass}}$

Low deposition rates

Ion-beam assisted deposition (?)

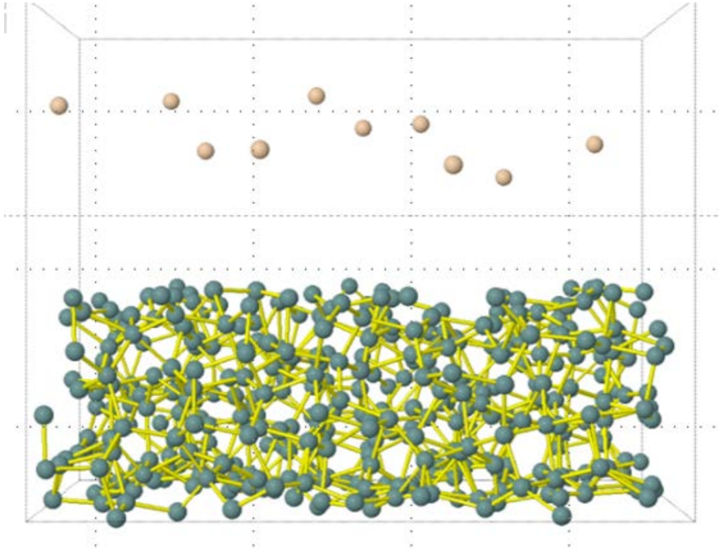
Applicable to amorphous oxides?

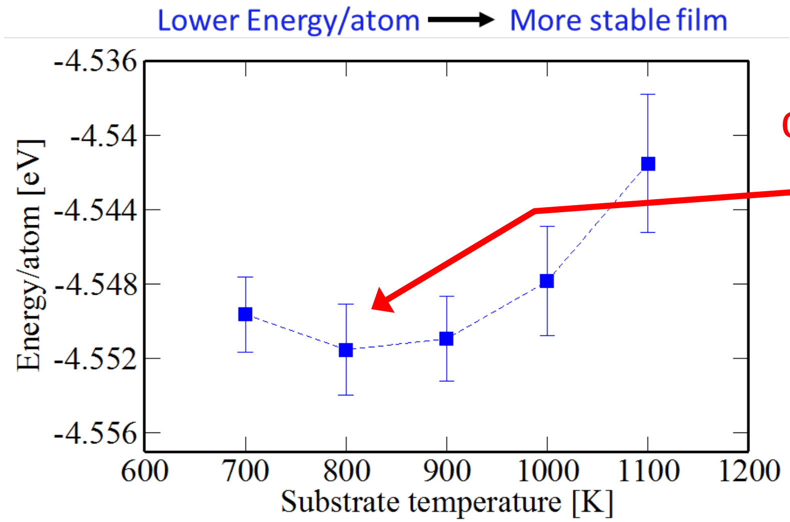


X. Liu, F. Hellman, et al, *PRL* **113**, 025503 (2014)

Amorphous silicon growth simulations

MD with classical potentials





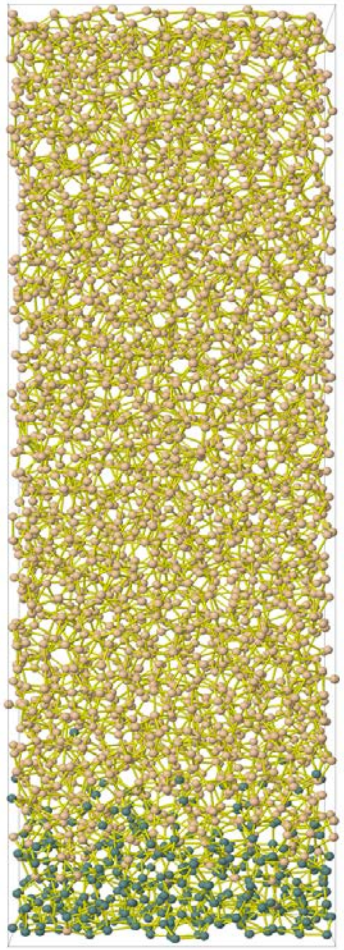
close to experimental (~750 K)

Test case for more complex materials (oxides)

Suggest suitable dopants

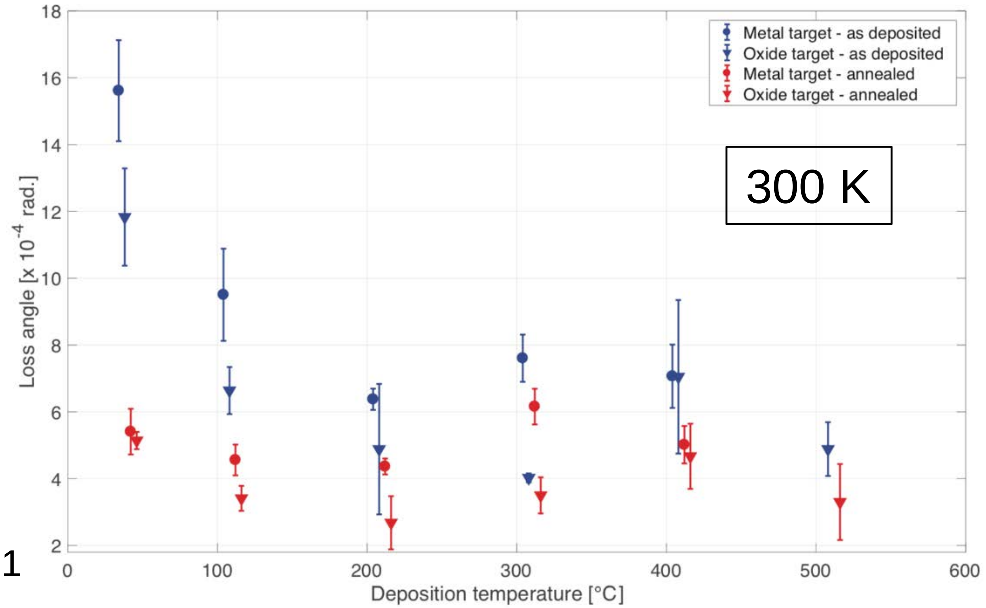
Guidance on optimum substrate temperature

preliminary



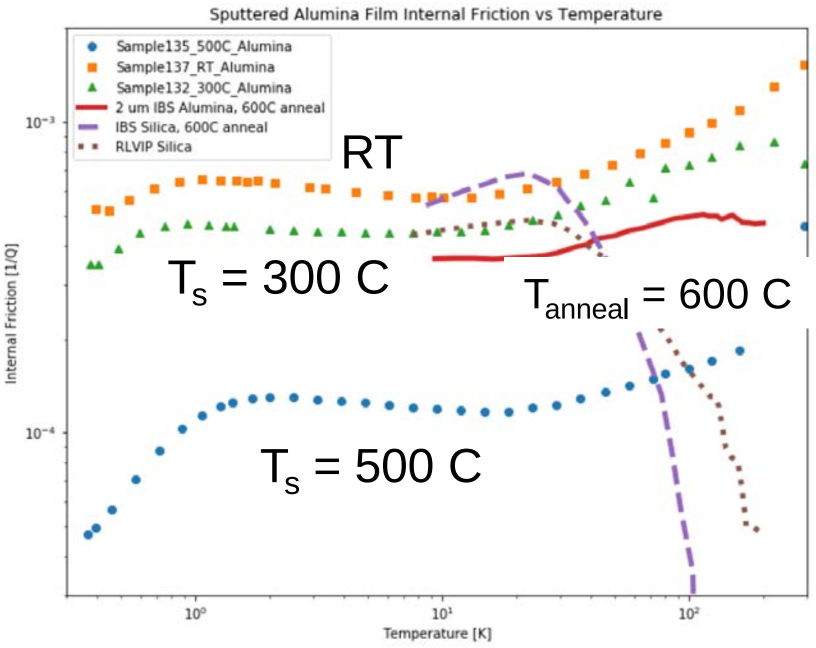
Ultra-stable Oxide Glasses?

- Ta_2O_5 high T_s deposition
  - lower loss than R.T. dep
  - but similar after annealing



G Vajente, (2018) Class. Quantum Grav. **35** 075001

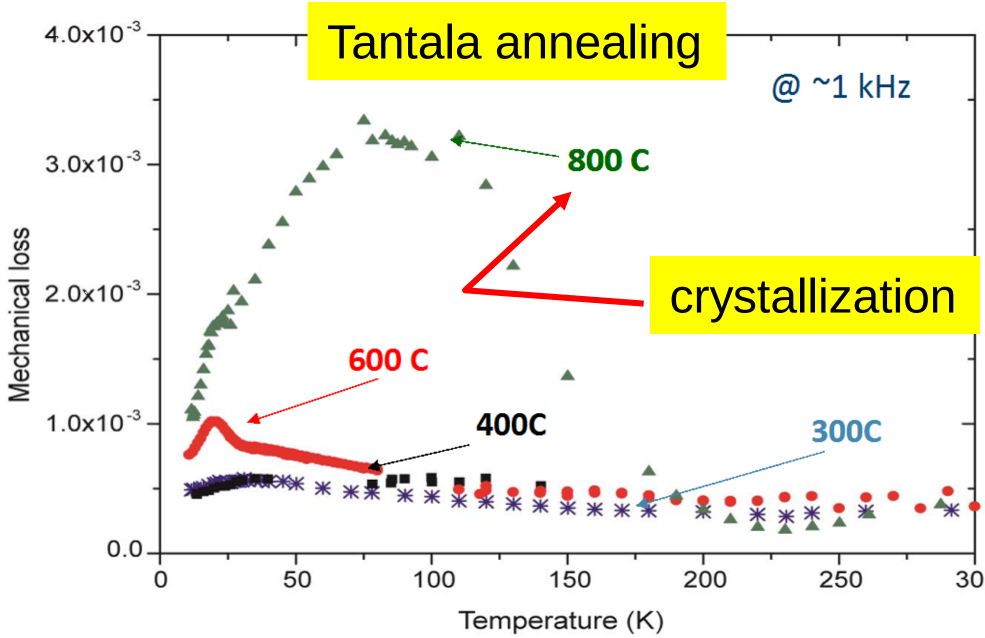
- Al_2O_3
  - cryogenic: better than SiO_2
  - preliminary: more characterization necessary
  - first ultrastable amorphous oxide?



M. Abernathy NRL LIGO G1800418

Suppressed Crystallization

- Annealing reduces R.T. loss ~monotonically with T_{anneal}
- Annealing temperature limited by onset of crystallization



Tantala annealing

crystallization

- Suppression of crystallization valuable path to low loss
  - chemical frustration

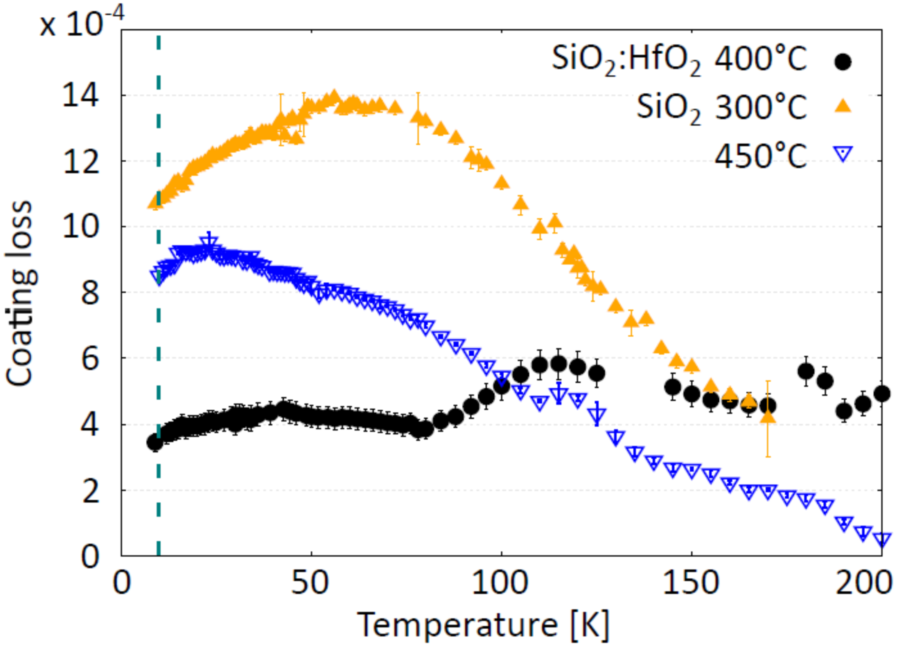
    suitable dopants: two cations ($Ti:Ta_2O_5$), three cations …
  - geometrical frustration

    nanolayers thinner than critical crystal nucleus

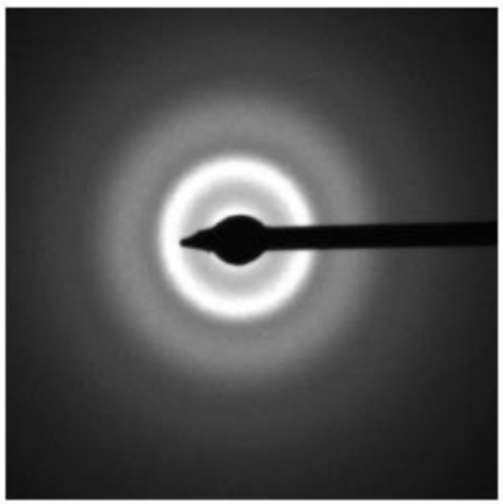
SiO_2:HfO_2

- 27%SiO_2:HfO_2
    - HfO_2 crystallizes as deposited
    - SiO_2 suppresses up to 600C anneal
    - no low-T loss peak (vs SiO_2)
    - 2 x less loss than SiO_2 at 20 K

- Revisit for 10 K low-index layer

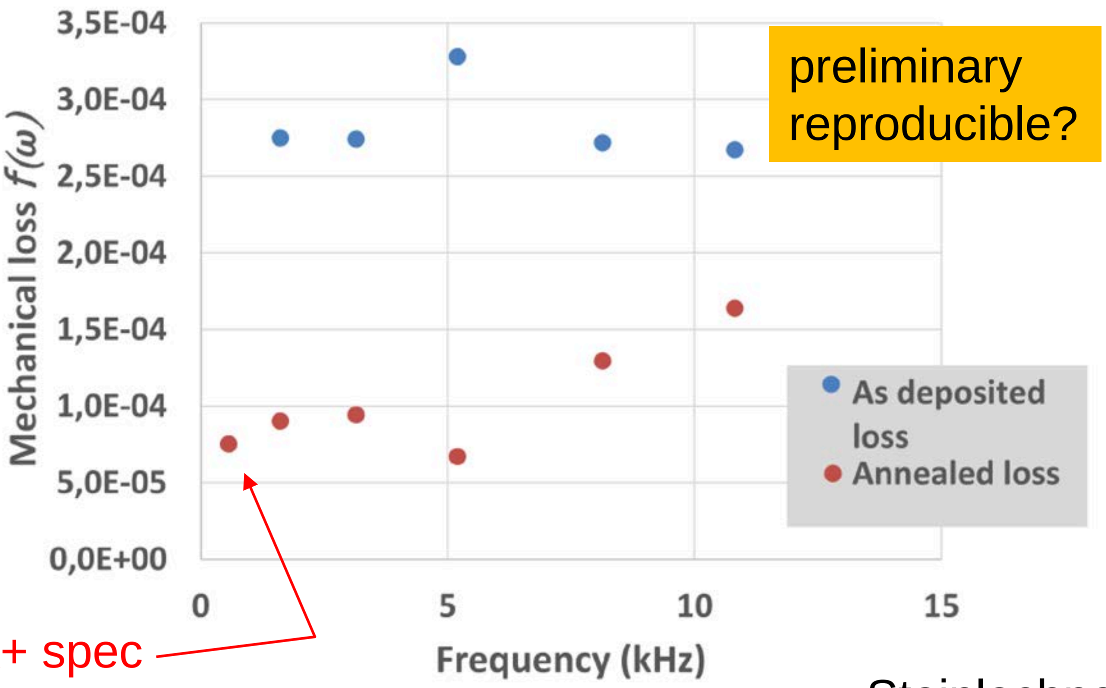


K. Craig et al, GEO, LIGO-P1800241



Annealing Mixed Oxides: Zr:Ta_2O_5

- Anticipate chemical frustration of crystallization in mixed oxides
- ~15%Zr:Ta_2O_5 shows promising results
  - low rate deposition (S. Reid with ECR)
  - no crystallization up to 750 C (compare ~600 C Ta_2O_5)



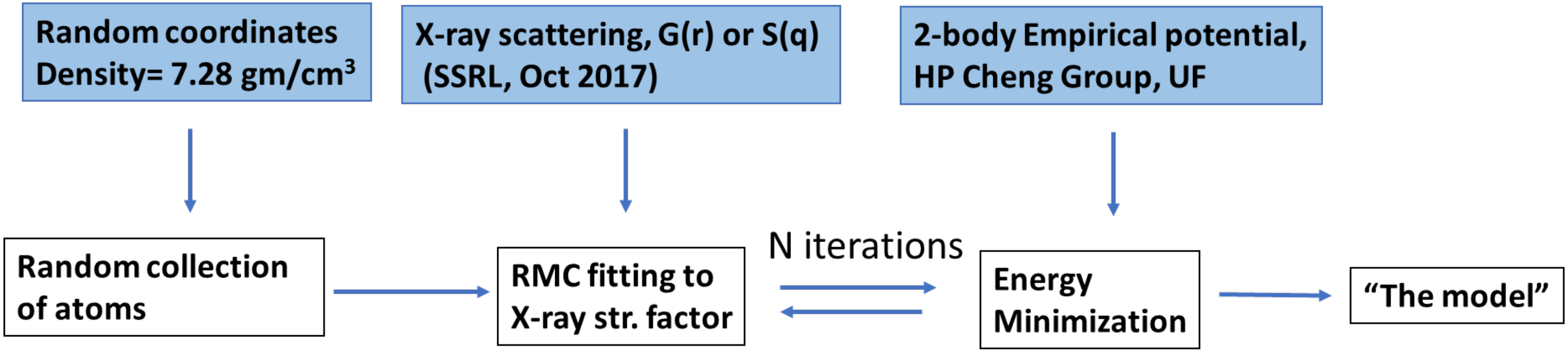
preliminary
reproducible?

approaching A+ spec

Steinlechner LIGO-G1800585b

  - IBS ~48%Zr:Ta_2O_5 up to 800 C (not as good as low-rate 15%Zr:Ta_2O_5)

Structure Determination from X-Ray Scattering



Random coordinates
Density= 7.28 gm/cm^3

X-ray scattering, G(r) or S(q)
(SSRL, Oct 2017)

2-body Empirical potential,
HP Cheng Group, UF

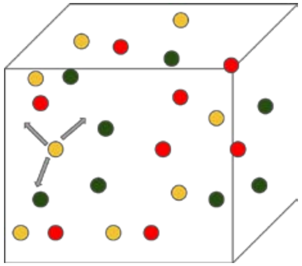
Random collection of atoms

RMC fitting to X-ray str. factor

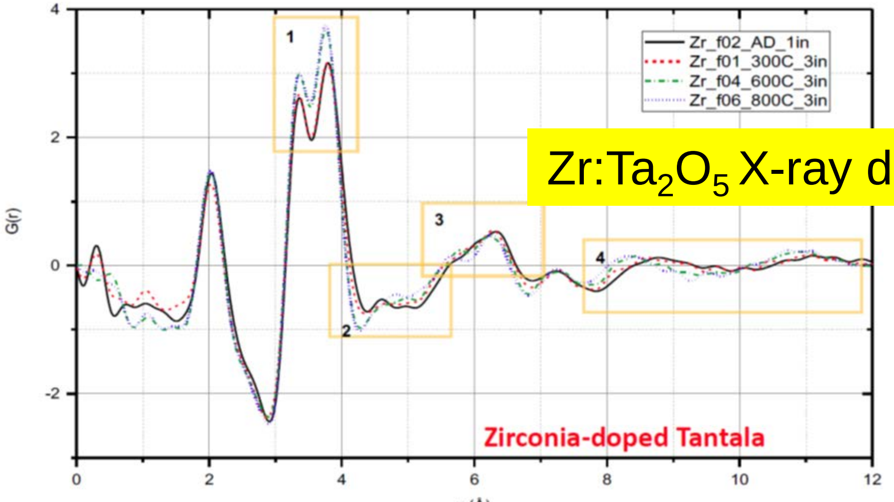
N iterations

Energy Minimization

“The model”



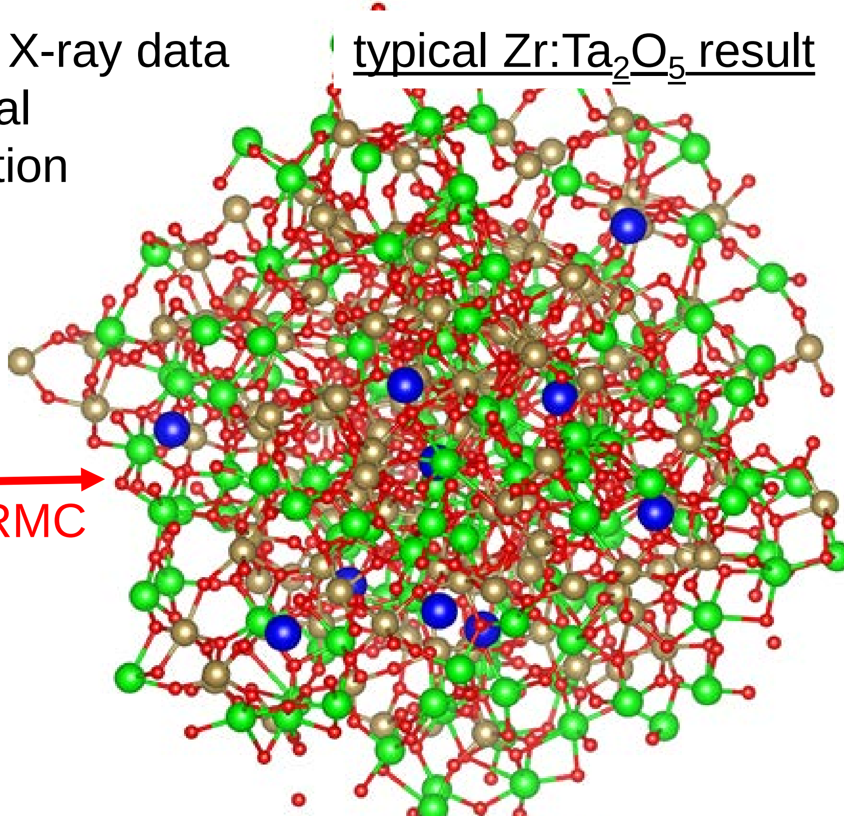
Reverse Monte-Carlo fitting to X-ray data constrained with experimental (RBS) density and composition



Zr:Ta_2O_5 X-ray data

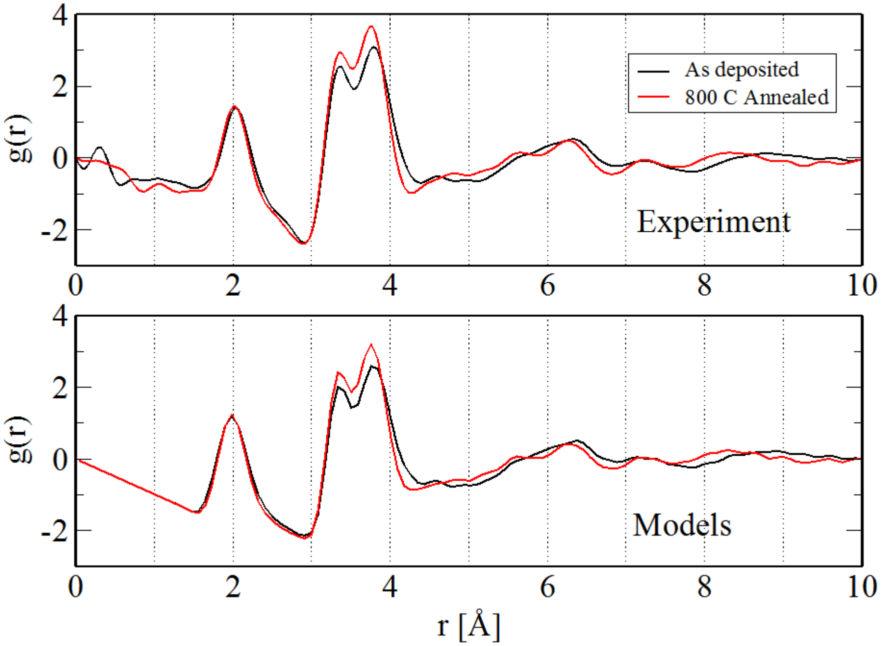
RMC

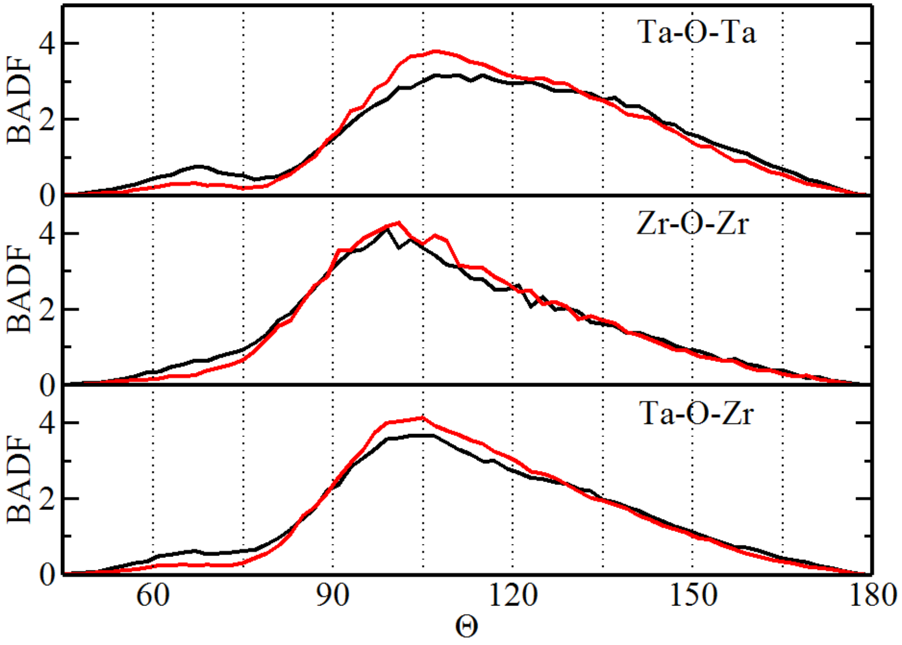
typical Zr:Ta_2O_5 result



Structural Characterization (Zr:Ta_2O_5)

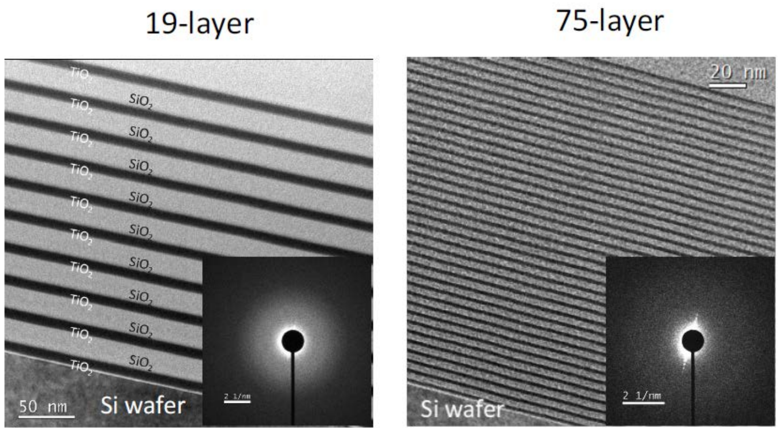
- Recovered models fit well to data
  - in both short and medium range order
- Clear narrowing of bond-angle distribution with annealing
  - possible connection to high vs low temperature behavior
- Currently computing predicted mechanical loss
  - and responsible motifs





Nanolayers

- Investigate silica with nanolayers of titania
  - NTHU LIGO-G1800300
  - different thicknesses, same ratio

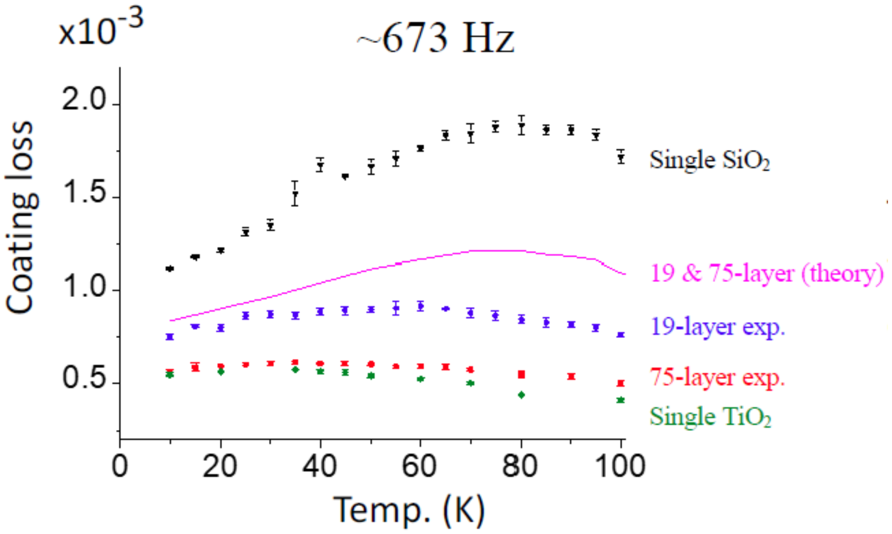


	thickness (nm)
SiO_2	19.3 ± 0.1 (x9)
TiO_2	8.3 ± 0.2 (x10)
$r = 0.32$	

	thickness (nm)
SiO_2	3.6 ± 0.1 (x37)
TiO_2	1.8 ± 0.1 (x38)
$r = 0.33$	

- Cryogenic loss peak suppressed

Low-temperature ϕ suppressed



- Also see crystallization suppression in TiO_2

Amorphous Oxides Take-Aways

- Theory ←→ atomic structure ←→ synthesis beginning to interact usefully
  - should speed navigation of experimental parameter space

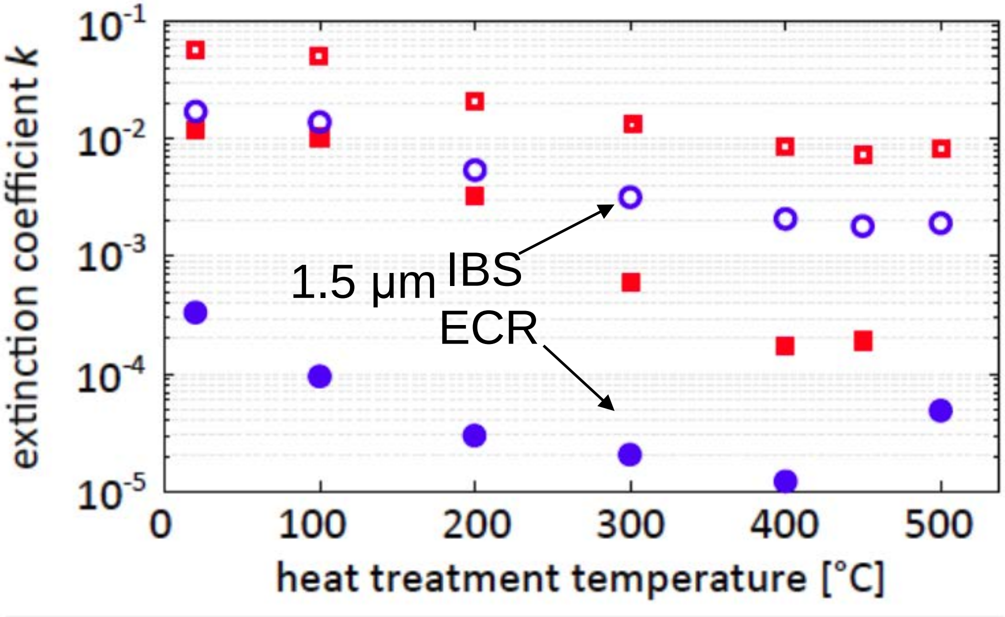
- Promising results on
  - ideal glass
  - crystallization suppression

- (preliminary) evidence of suitable materials for A+
  - not yet fully reproducible

- Non-trivial development time after down-select material
  - depends on how far deposition method is from conventional IBS

Amorphous Semiconductors for Cryogenic Mirrors

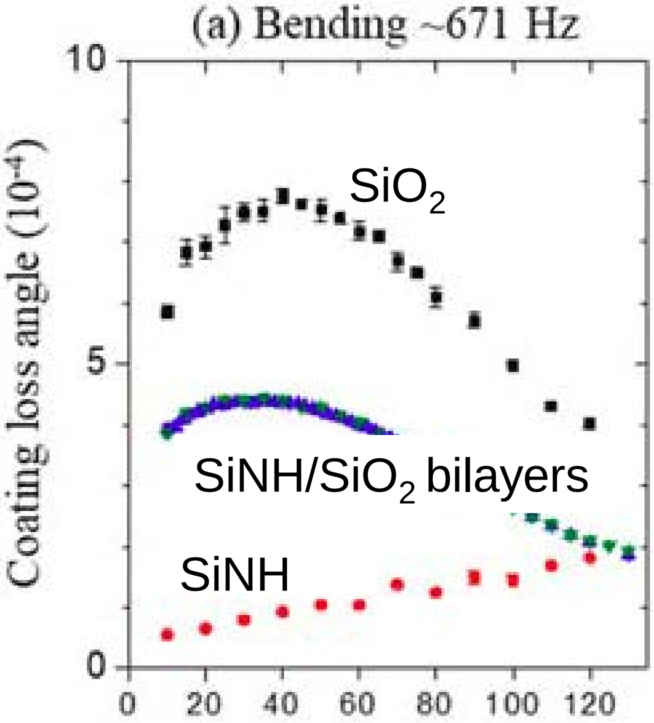
- Mechanical properties adequate
  - problems from optical absorption
  - worse at 1 μm → 1.5 μm → 2 μm
- a-Si
  - low-rate ECR deposition
  - 100-fold optical absorption reduction vs conventional IBS
  - add hydrogen annealing?
- a-Si/SiO_2 HR: ~10 ppm abs.
  - apply in MMC



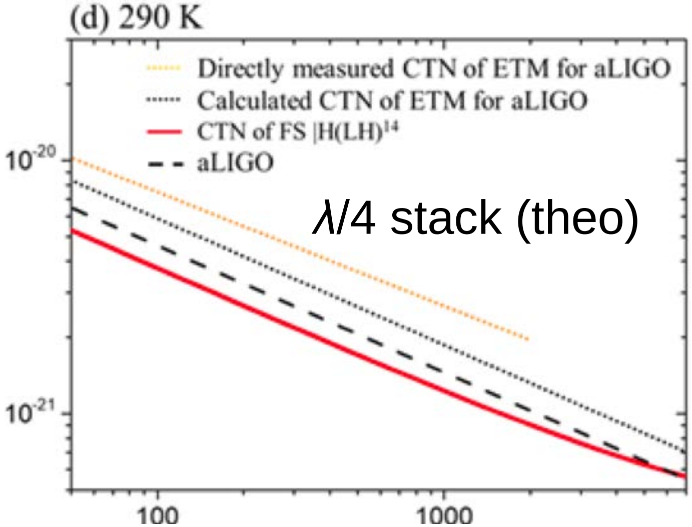
Birney, **LIGO-G1801091-v1**

Silicon Nitride

- LPCVD deposition of $SiN_{0.40}H_{0.79}$
  - R.T.: ϕ ~1 x 10^{-4}
  - no low temperature loss peak
- 1/4-wave $SiN_{0.40}H_{0.79}/SiO_2$ bilayers
  - within ~2 of ET-LF and Voyager CTN specs
- Optical absorption of SiN/SiO_2 HR: ~50 ppm
  - requires multi-material coating with Ta_2O_5/SiO_2
  - can bring absorption to ~2 ppm
- Annealing behavior studies underway



(a) Bending ~671 Hz

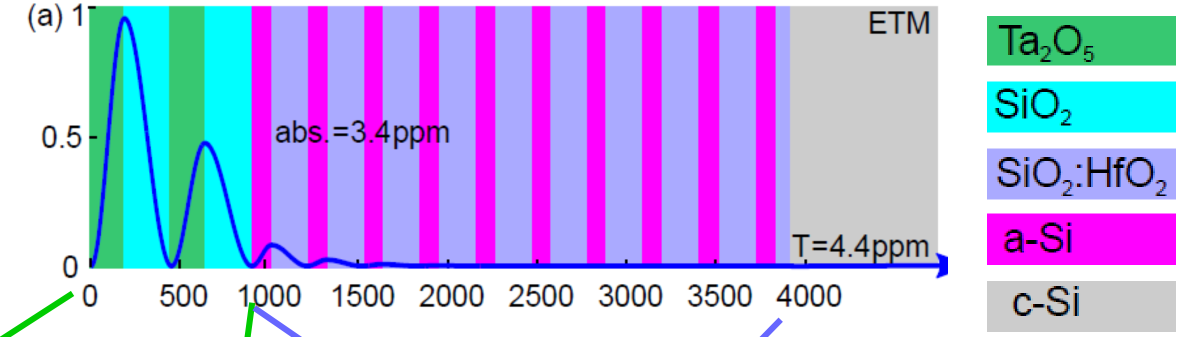


(d) 290 K

Pan et al NYHU, P1800164-v3

Mix and Match for Cryogenics

- Adequate elastic losses available for cryo operation
  - – issue in all cases is associated optical absorption
- Multi-material coatings (MMC) a possible solution



Low optical loss
High elastic loss

Ti:Ta_2O_5
SiO_2
improved oxides

High optical loss
Low elastic loss

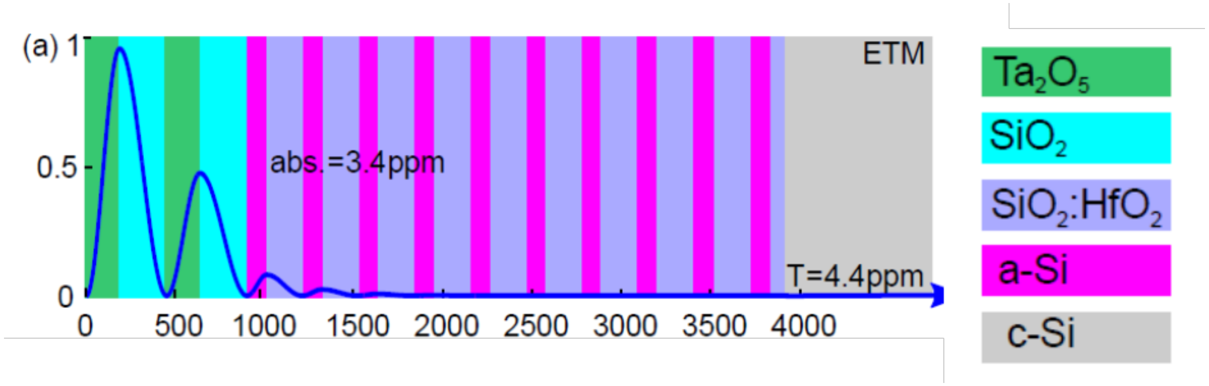
a-Si
SiNH
SiO_2:HfO_2
High-T Al_2O_3?

I.Martin LIGO-G1801548

Can trade one misbehavior for the other

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

10 K Example

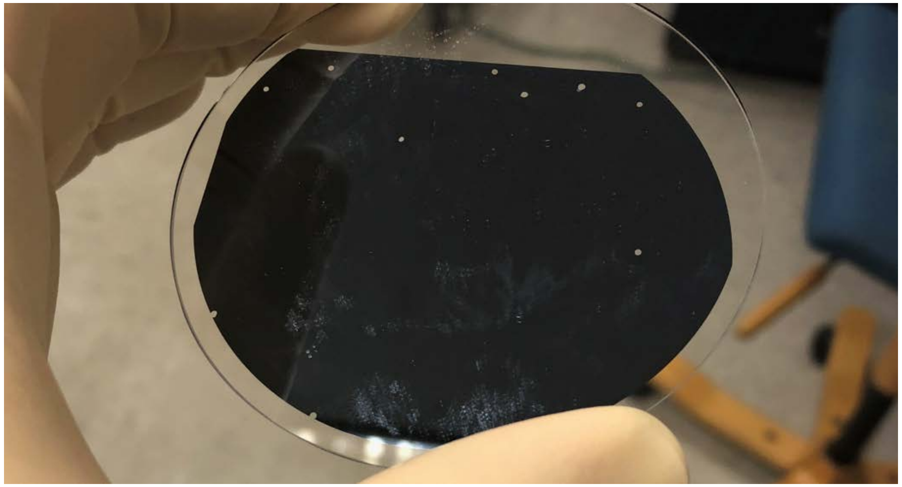


Case	bilayers ETM (ITM)	Transmission ETM (ITM) [ppm]	Heat treatment [°C]	CTN ETM (ITM) [$\times 10^{-21}$ m/$\sqrt{\text{Hz}}$]	CTN$_\text{D}$	α_HR [ppm]
Conventional	18 (7) × SiO_2/Ta_2O_5	4 (8500)	600	3.9 (2.3)	6.5	0.6
a-Si	10 (4) × SiO_2:HfO_2/a-Si	2 (9000)	400	1.4 (0.9)	2.4	11.9
a-Si MMC	SiO_2/Ta_2O_5 + 10 (4) × SiO_2:HfO_2/a-Si	4.4 (6000)	400	1.9 (1.5)	3.4	3.4
ET-LF requirement [12]		5 (7000)			≈ 3.4	≤ 5

K. Craig, P1800241-v2

Crystalline Coatings

- Absorption and mechanical loss OK for all applications
  - scatter statistics need further characterization
  - uniformity over larger areas



- Scaling to suitable dimensions
  - G. Cole: ~$40M (GaAs substrate + MBE + bonding tool)
- Note also environmental and thermodynamic tolerances
  - via electro-optic and piezoelectric effects

    1 V/cm $\rightarrow$ ~50 nrad Δ reflection phase
  - needs further study

Some Key Decision Aspects

- Timelines to select material system
  - A+LIGO: 2 years
  - cryogenic (Voyager, ET LF): > 5 years
- Research approaches
  - 300 K, 1 μm: amorphous oxides

    optical ok, elastic needs work
  - cryogenic, 1.5 – 2 μm, amorphous (crystal?) semiconductors, MMC

    elastic ok, optical needs work
- Tooling
  - only LMA IBS system currently can meet optical specs

    compatible with low rates, semiconductor materials?
  - other deposition methods require tool development ($$, time)

    ECR sputter: low rate oxide and a-semiconductor

    LPCVD: amorphous semiconductors

    crystal growth + MBE + bonding: AlGaAs crystal mirrors
  - how/when to begin to develop alternative tools?

Path(s) Forward for Cryogenic 3G Coatings

As simple as it can be, but no simpler

- Amorphous semiconductors
  - continue to explore parameter space to reduce absorption

    rate, temperature, annealing temperature and atmosphere

- Multi-material mirrors
  - test optical properties and thermal noise on complete HRs
  - explore alternative low-index oxide layers

    nanolayers to suppress crystallization/loss?

- Alternative deposition methods to IBS
  - low-rate ECR, LPCVD

    better material properties obtained than IBS

  - realistic for scaled-up mirrors?

    fab small HRs, evaluate scatter etc

    evaluate tooling cost (and time) to adapt to 3G-scale mirrors

Path(s) Forward for Cryogenic 3G Coatings

- Crystalline mirrors
  - best absorption and thermal noise combination
  - more complete scatter statistics useful
  - electro-optic and piezoelectric properties
    - evaluate thermodynamic and environmental implications
  - scaling expensive