Modeling and simulations of amorphous coatings

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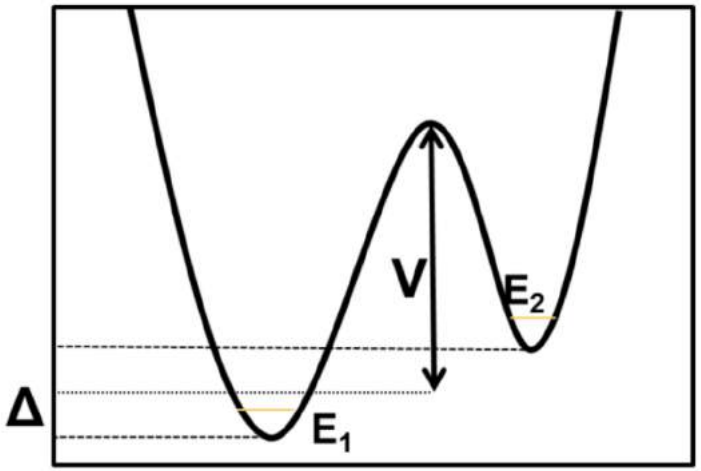
GORDON AND BETTY MOORE FOUNDATION

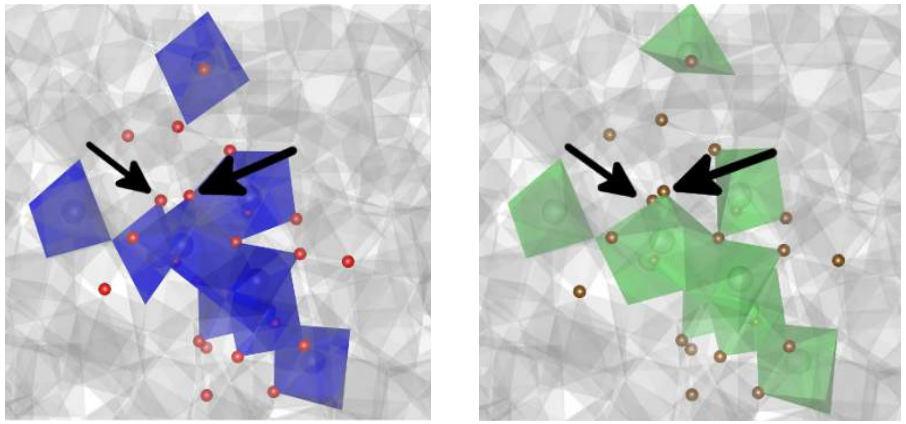
Overview

- The optical coatings in the current LIGO mirrors use **amorphous** materials



- Reducing thermal noise comes down to **reducing two-level systems** that are intrinsic to amorphous coatings

- Some successes are coming from:
  - Choice of coating materials
  - Elevated temperature deposition: mainly in *a*-Si
  - Post-deposition annealing
  - Doping material/percentage
  - Nano-layering



TLS in *a*-Ta_2O_5
Trinastic, PRB **93**, 014105 (2016)

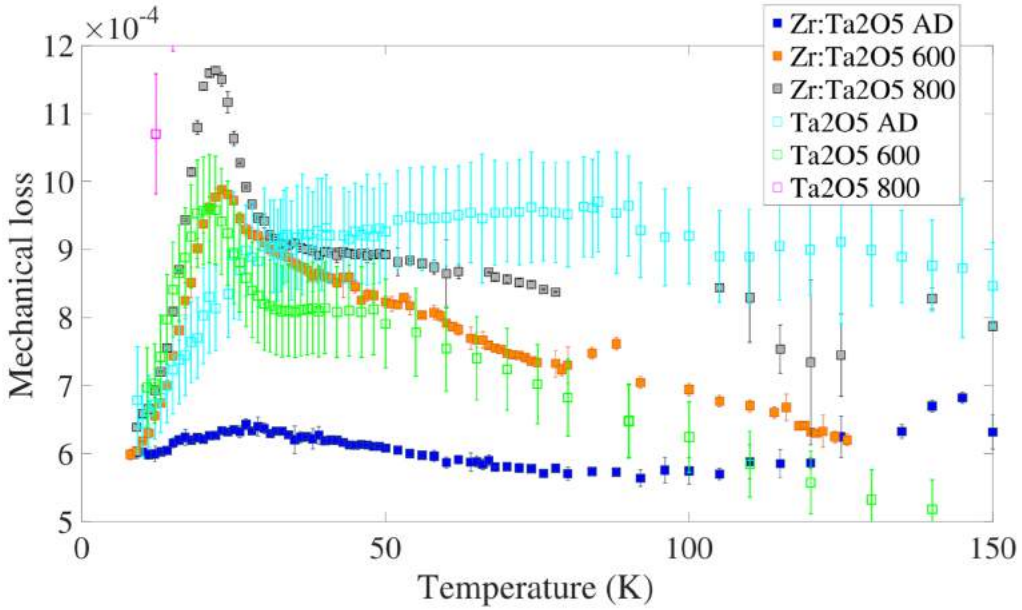
Plan of this talk

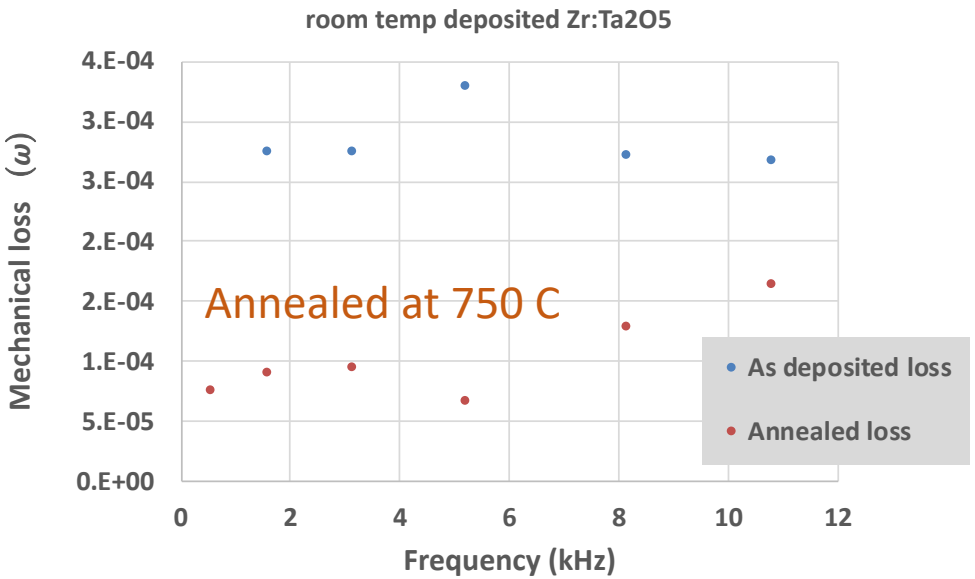
- Zirconia-doped-Tantala
  Insights from structural characterization

- Amorphous Si
  Vapor deposition simulations

Zirconia-doped-Tantala

- Measured loss at room temperature decreases with annealing at higher temperatures





Source for both figures: G1800585-v3

- Doping with Zirconia suppresses crystallization:
  makes higher temperature (up to 900 C*) annealing possible

*According to G1800585-v3

Pair Distribution Function (PDF)

- **Pair Distribution Function:**
  Average position of atoms

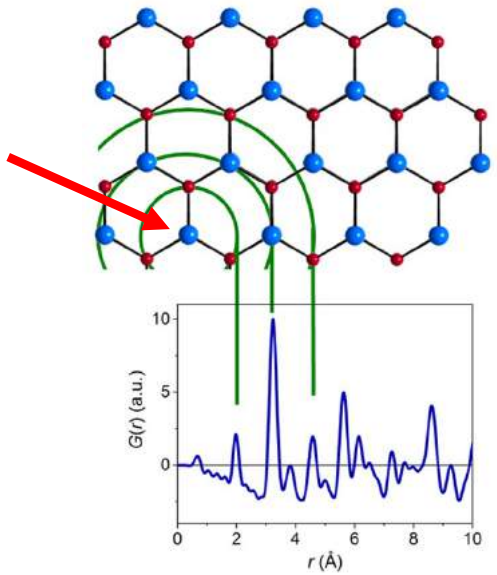
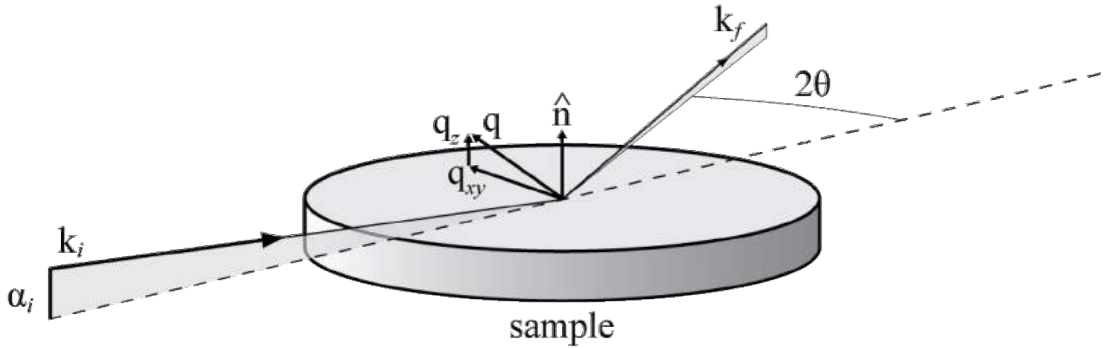


Figure: 2D Crystal for illustration

- **Connecting link between experiments and modeling**

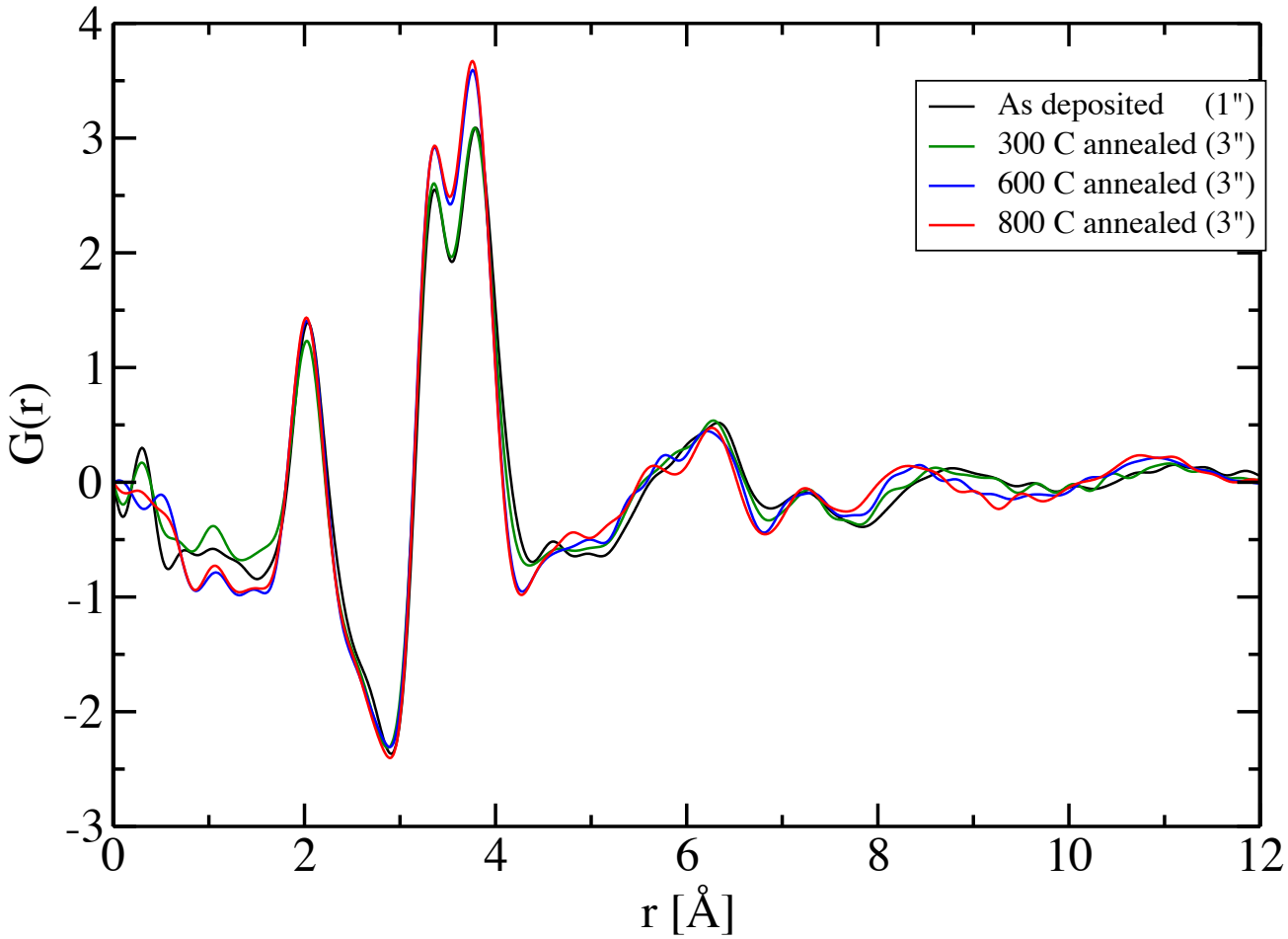
- **Experimentally measured as**
  Grazing Incidence Pair Distribution Function (GIPDF)



$$G(r) = \frac{1}{(2\pi)^3 \rho_0} \int_0^\infty 4\pi Q^2 F(Q) \frac{\sin Qr}{Qr} \, dQ$$

Figure source: https://en.wikipedia.org/wiki/Grazing_incidence_diffraction
Figure source: http://www.mesostructures.uni-bayreuth.de/en/research/pair-distribution/index.html

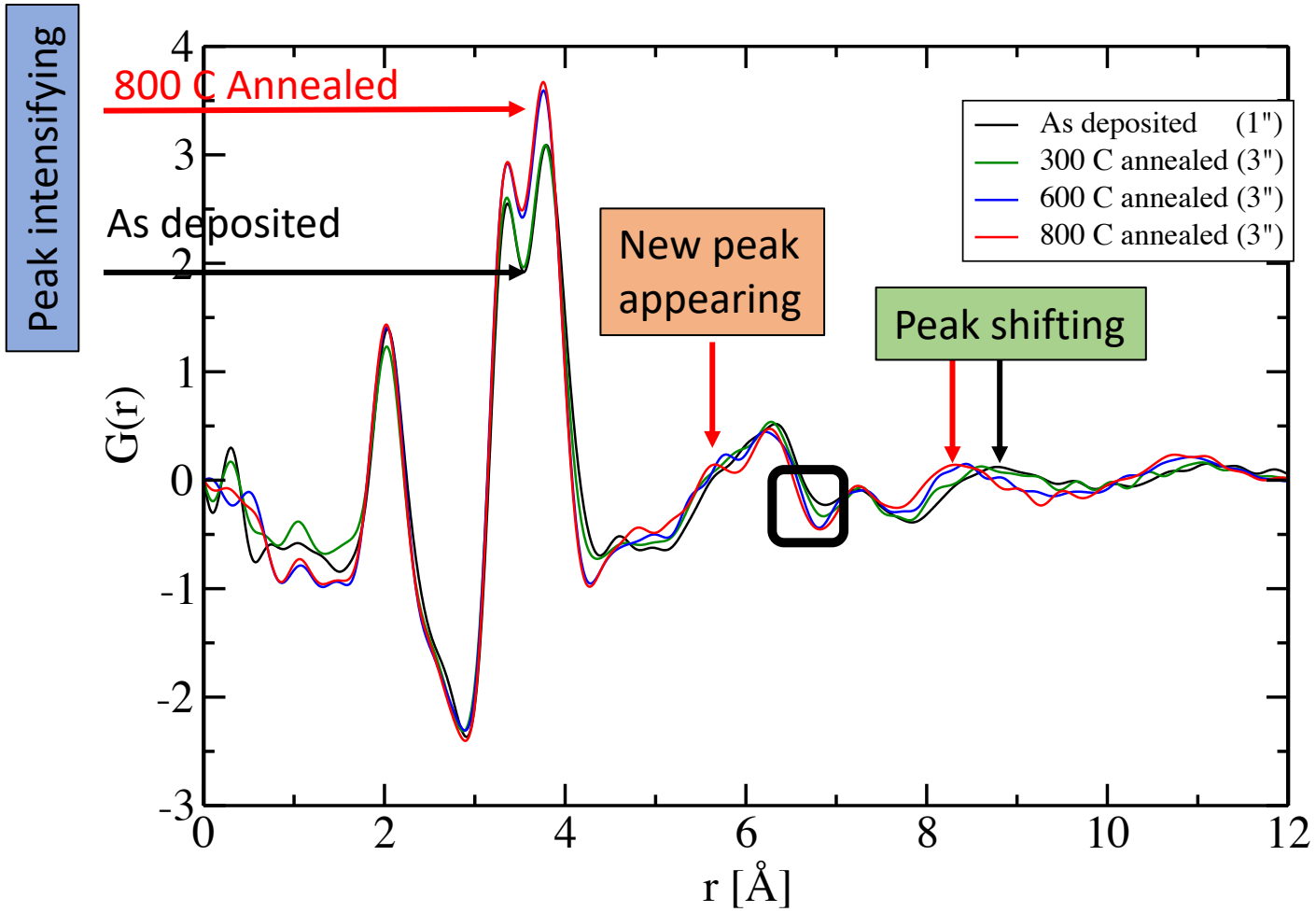
Measured PDF of Zirconia-doped-Tantala

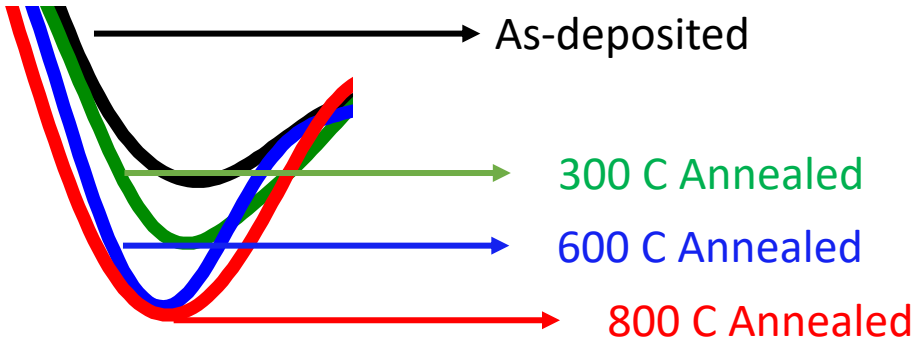


X-Ray GIPDF measurement on 35% Zirconia-doped-Tantala

SLAC National Accelerator Laboratory, October 2017

Measured PDF of Zirconia-doped-Tantala

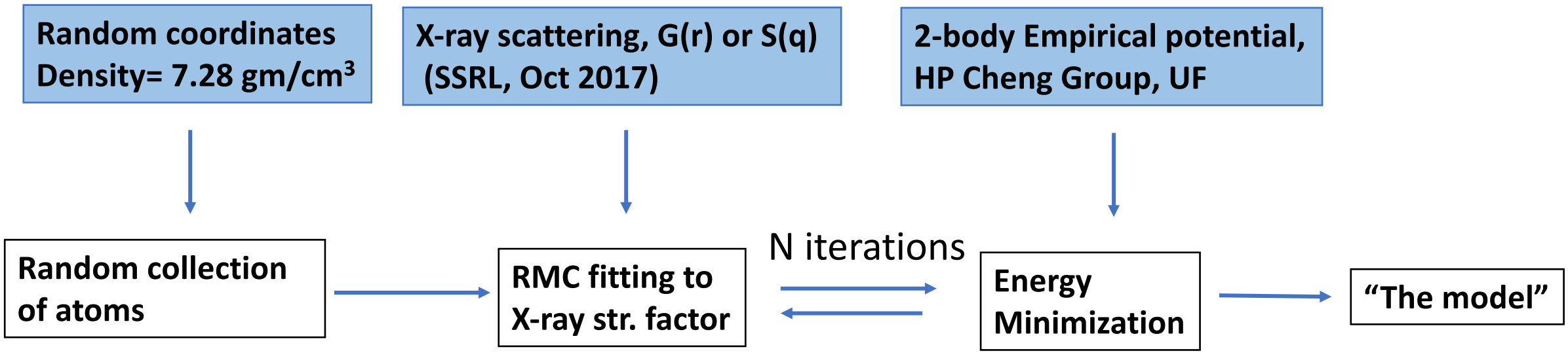




X-Ray GIPDF measurement on 35% Zirconia-doped-Tantala

SLAC National Accelerator Laboratory, October 2017

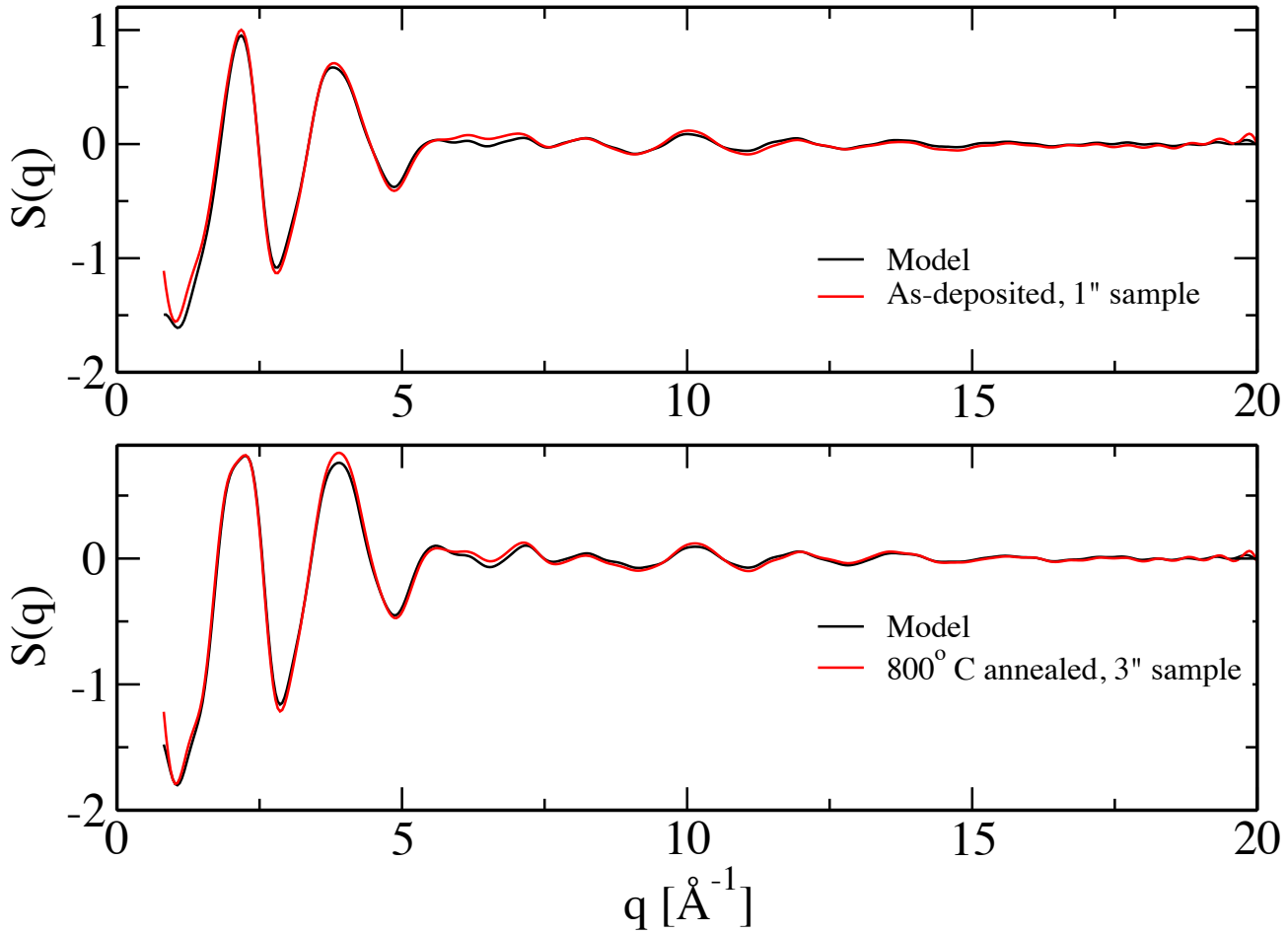
Modeling of Zirconia-doped-Tantala

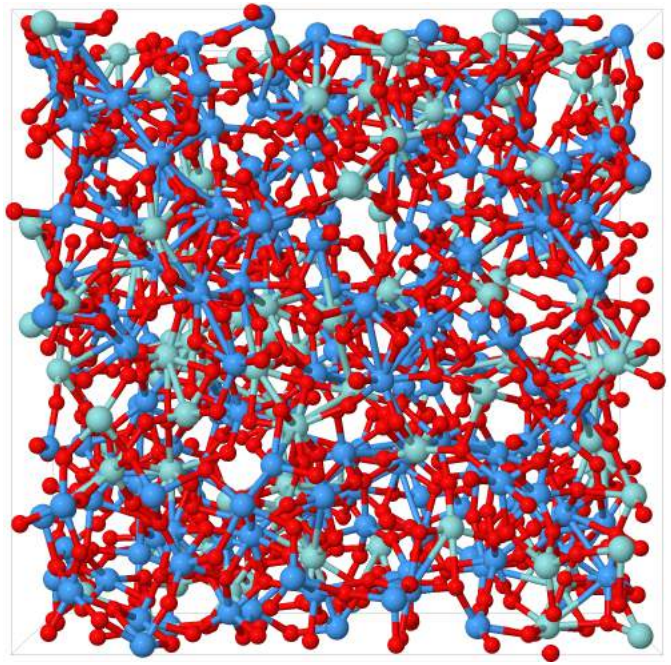


- 1064 atoms in all models,
- All results are averages over 100 models
- Density inferred from potential (Density measurements are underway!!)
- Fitting and minimization method:
  FEAR, Pandey, Biswas and Drabold, Scientific Reports **6:33731**, 2016

Modeling of Zirconia-doped-Tantala

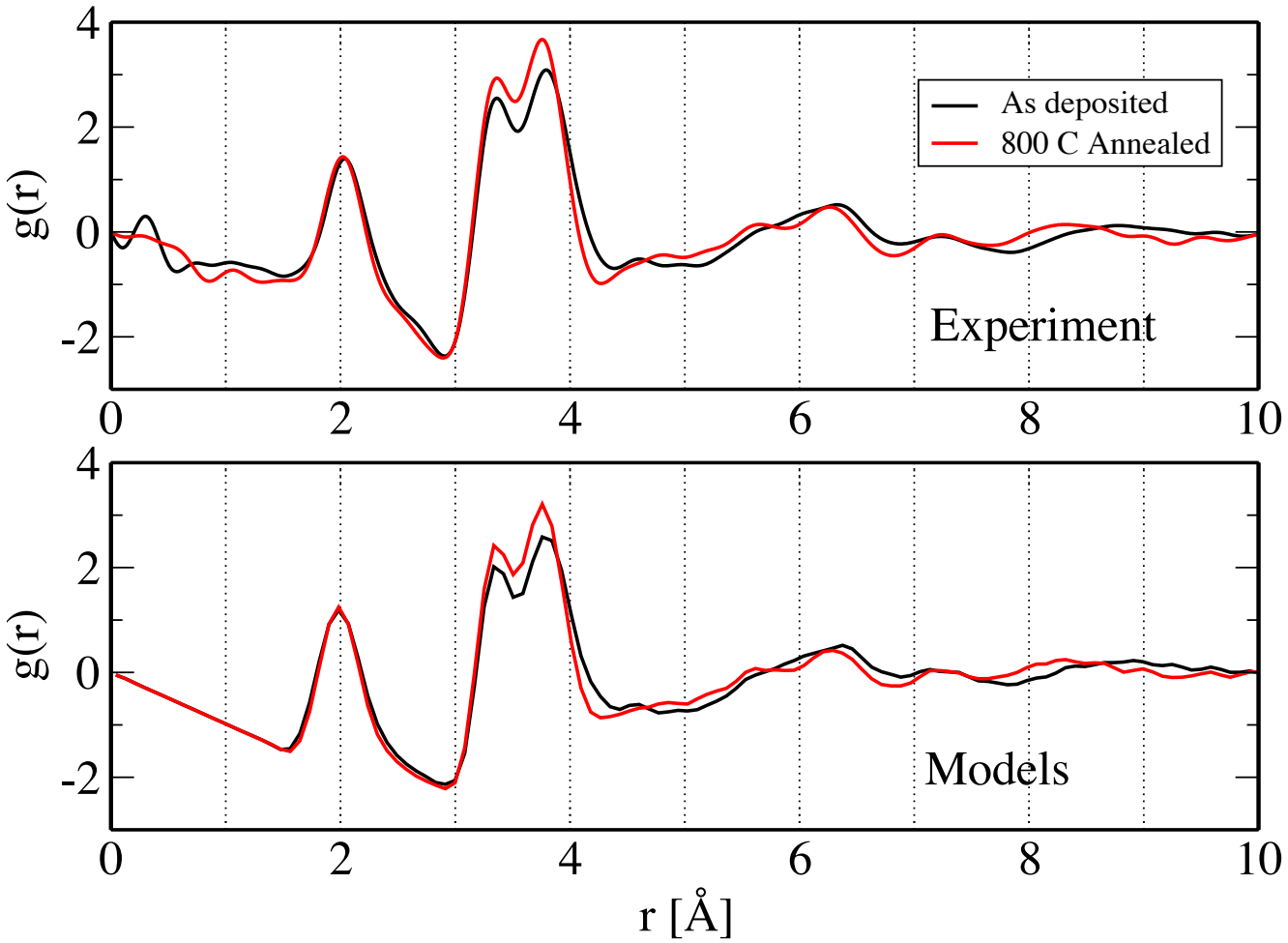
Atomic models fitted to x-ray structure factor S(q)





Ball and Stick representation of final model

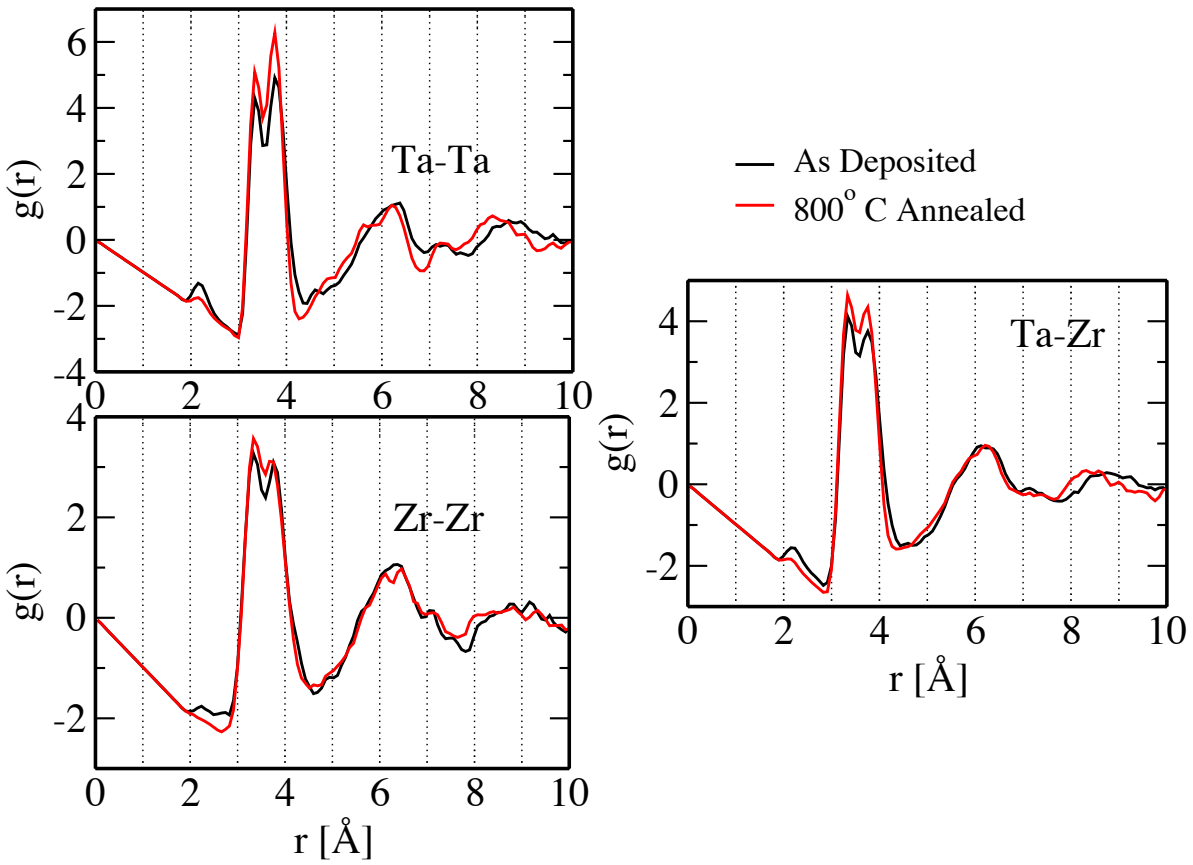
Modeling of Zirconia-doped-Tantala



Models track the changes in experimental PDF very well

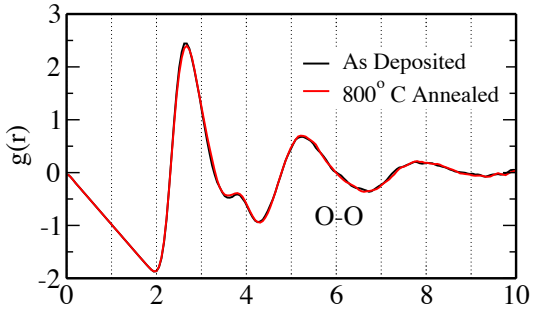
Modeling of Zirconia-doped-Tantala

Partial pair correlation functions

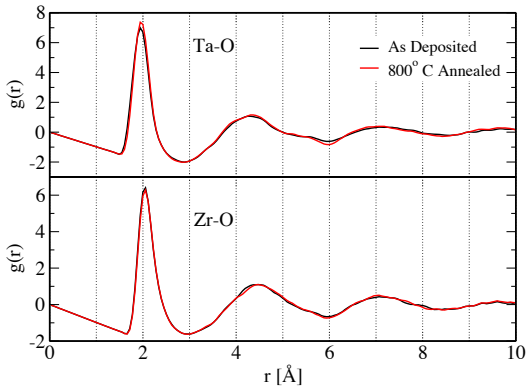


Effect of annealing in Metal-Metal correlation

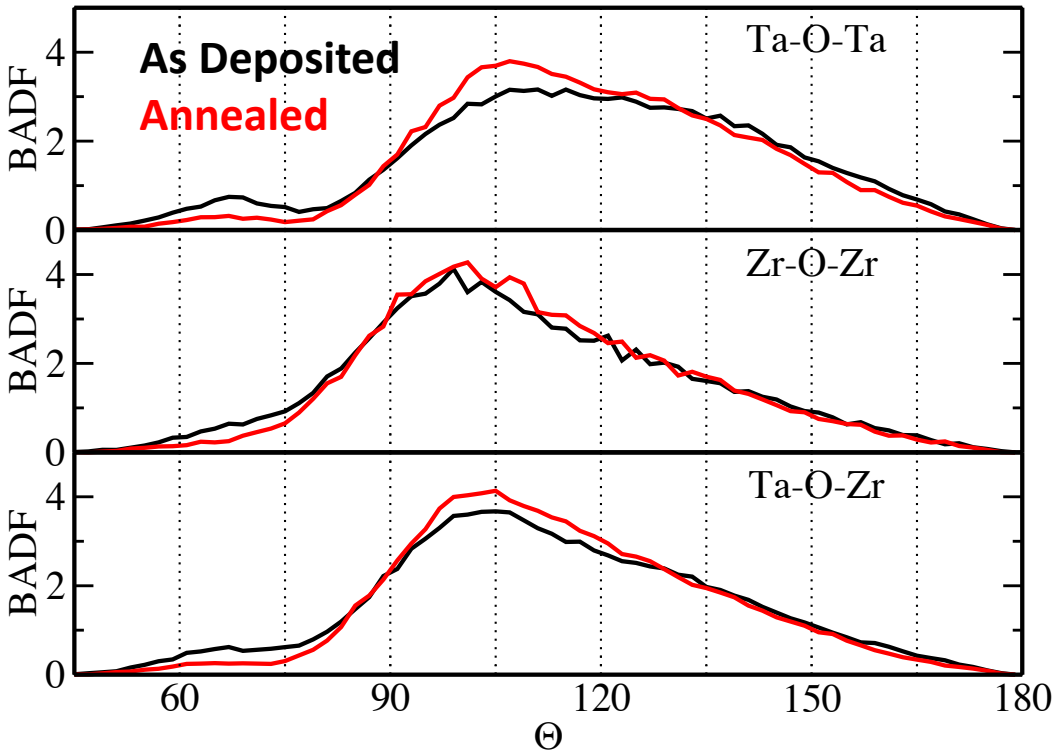
No major change in O-O correlation upon annealing.



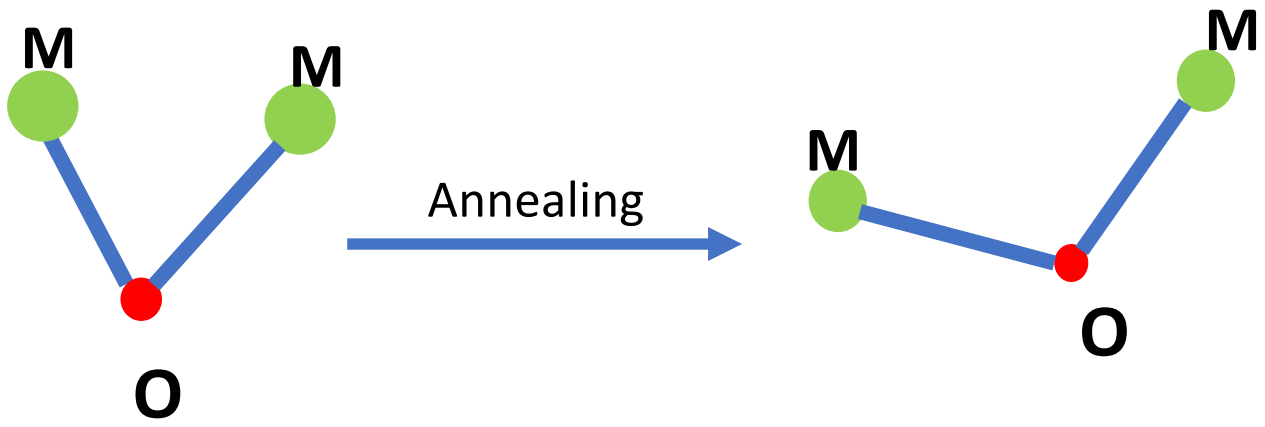
No major change in M-O correlation upon annealing.



Modeling of Zirconia-doped-Tantala



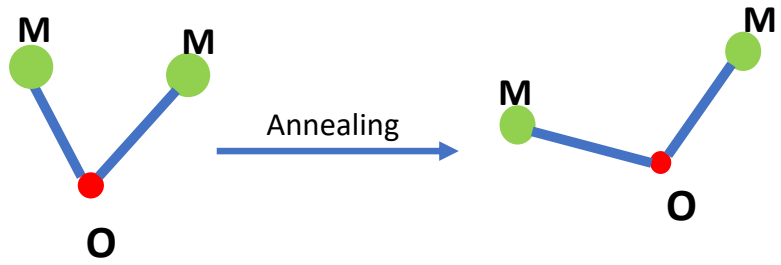
A simplified picture:

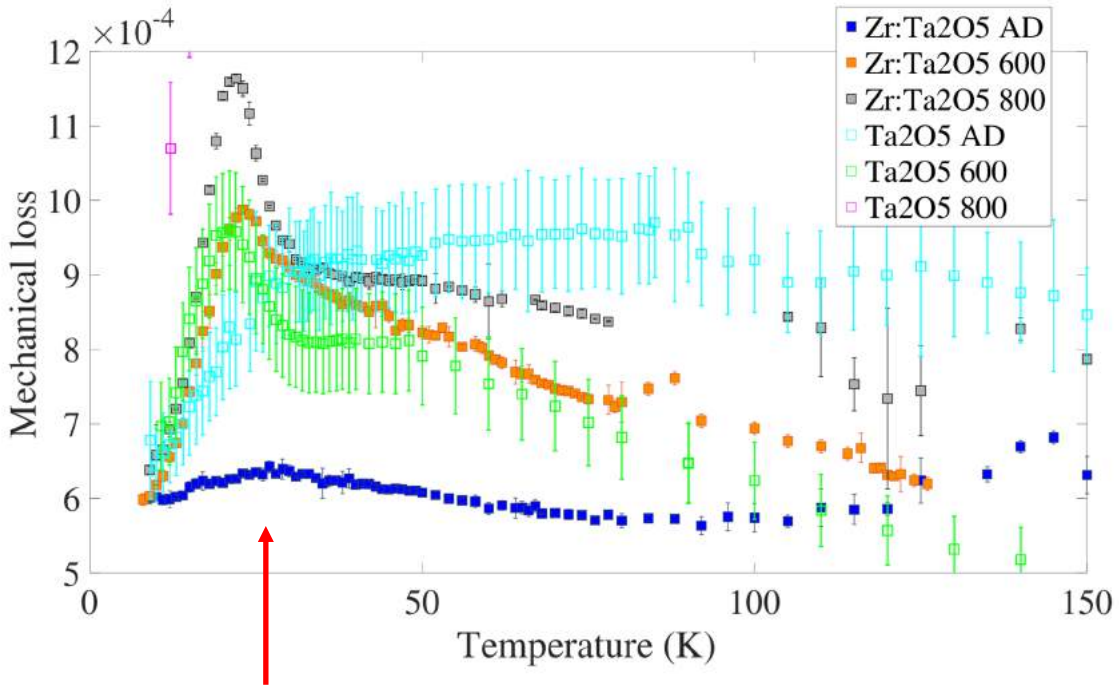


Bond angle distribution shows changes in M-O-M angles

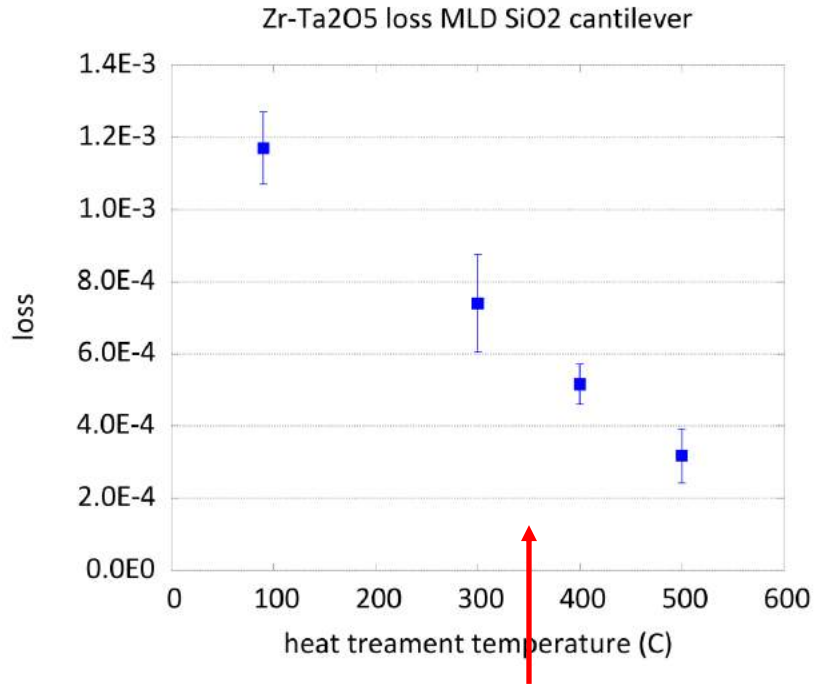
Modeling of Zirconia-doped-Tantala

Loss mechanism hypothesis:
(Needs validation from two-level system analysis)





Low barrier TLSs increase upon annealing



High barrier TLSs decrease upon annealing

Source of both plots: G1800585-v3

(More recent loss data exists!!)

Modeling of Zirconia-doped-Tantala

Next steps:

- Compute two-level systems and calculate mechanical loss
  (Team @ University of Florida is working on it!!)

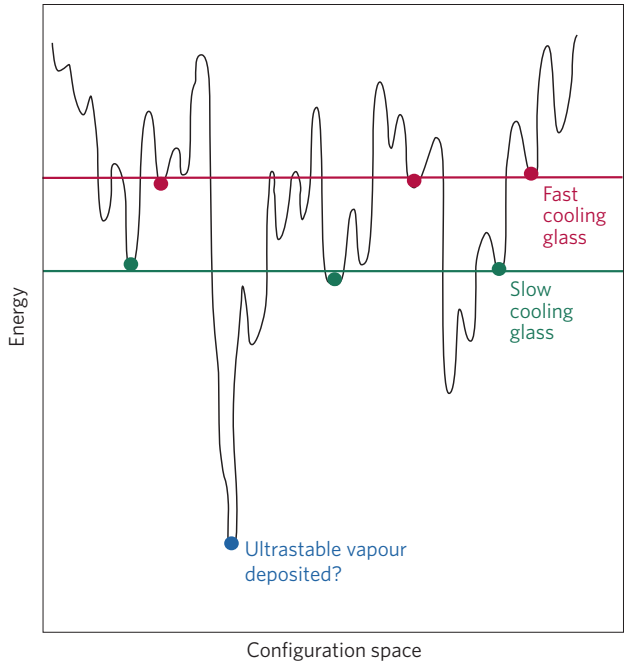
  See if the loss hypothesis holds.

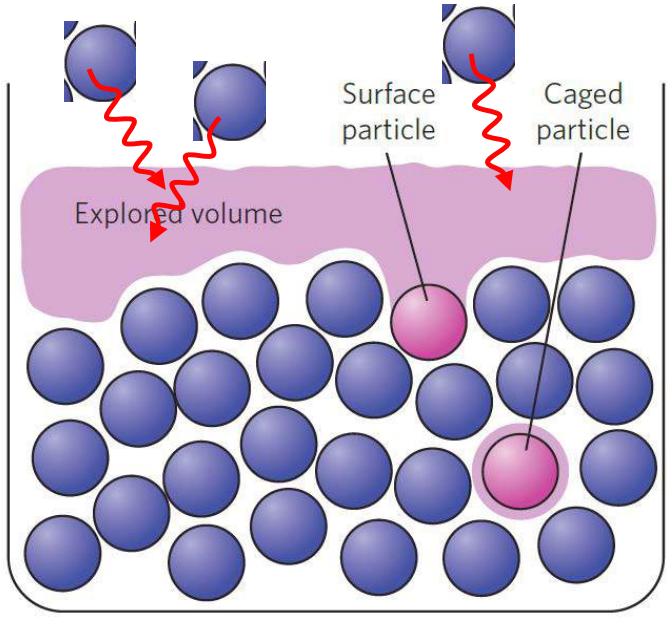
- Search for dopants that can frustrate the two-level dynamics

- Continue study how ZrO_2 doping inhibits crystallization in Ta_2O_5-
  Initial results from caloric curve analysis consistent with observed frustration of crystallization by ZrO2 doping

Vapor deposition simulations

- Vapor deposition simulations mimic the coating deposition process





Figures from: Nature Mater. 12, 94 (2013)

- Aim: simulations can identify advantageous materials, dopants, substrate temperature, deposition rate

Amorphous silicon

Why choose a-Si for growth simulation?

☛ Ideal test case for vapor deposition simulation

- Clear evidence of reduction in loss from experiments: E-beam deposited a-Si shows large drop in internal friction with high $T_{substrate}$ deposition
- Single atom type
- Interatomic potentials for a-Si are more mature than those for oxides

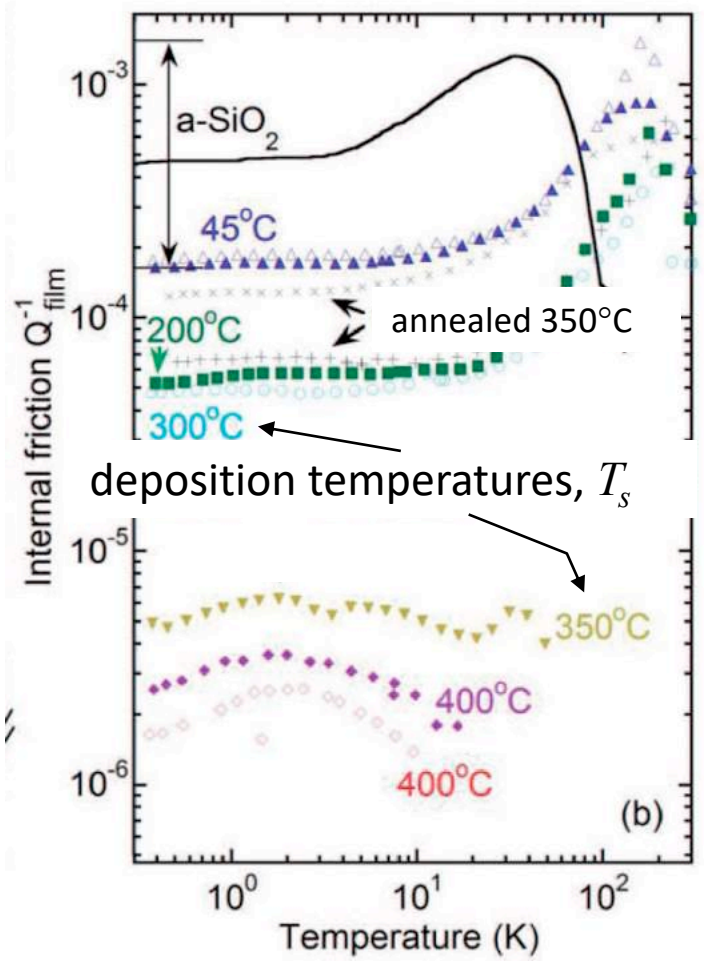
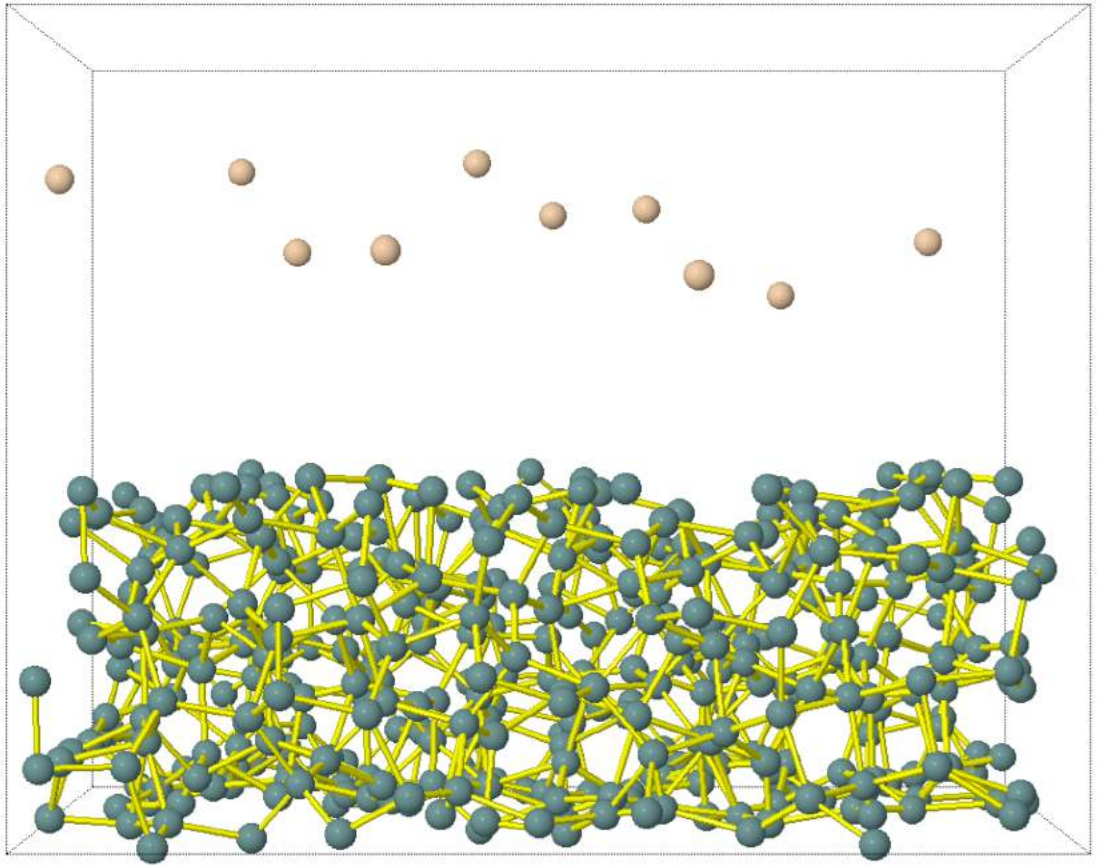
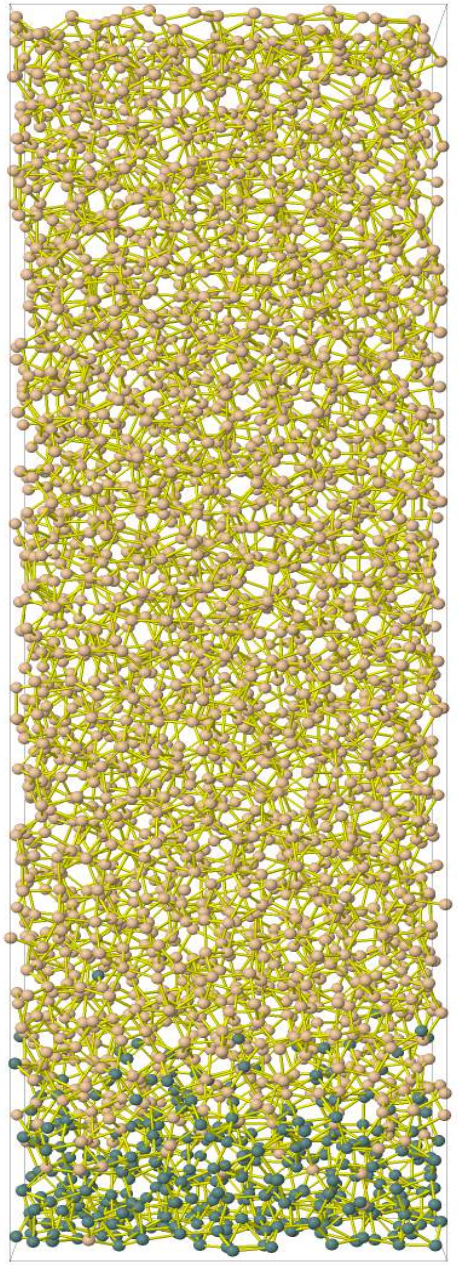


Figure reference:
Liu et al, PRL **113**, 025503 (2014)

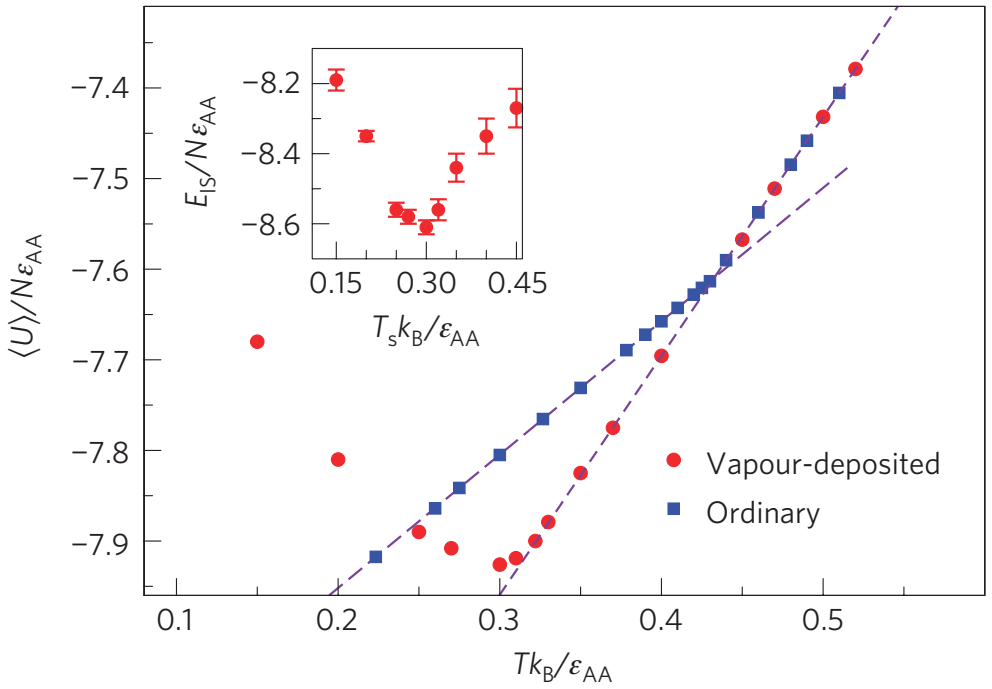
Amorphous silicon growth simulations





Amorphous silicon growth simulations

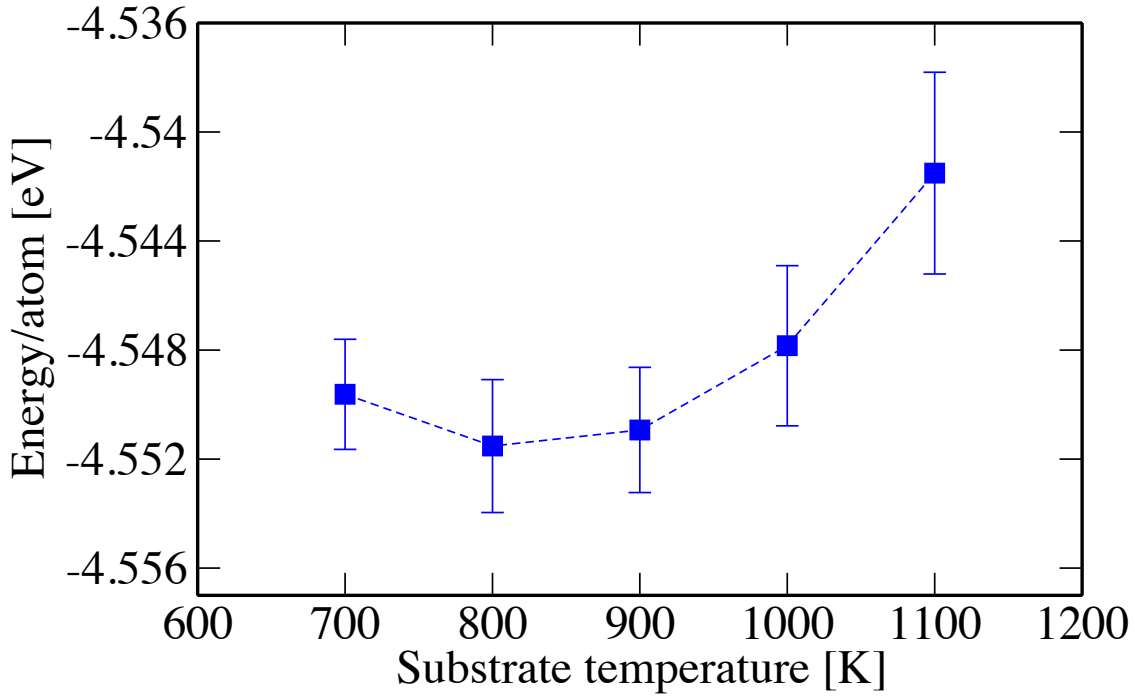
Sweet spot for $T_{substrate}$: 85% of T_{glass}?



Binary Lennard-Jones system

Source: Nature Materials **12.2** (2013)

Lower Energy/atom → More stable film



Amorphous silicon

Next steps: growth simulations

- Employ more accurate potential: Machine-learning based potentials are now available which are accurate as first principle calculations but scale ~N in computational cost (*Bartók, Kermode, Bernstein and Csányi, arXiv:1805.01568*)

- Characterize models: voids, density profile, rings distribution, two-level systems and mechanical loss

- **Extend the simulations to oxides**
  To model doping, substrate temperatures, mechanical loss and identify lower loss coatings

Summary

- X-ray scattering experiments have shown **clear trends of changes in short and medium range order** in the coatings with annealing.
- We have computer **models of coatings that capture the changes seen in samples** with annealing.
- Models indicate that **strained M-O-M bonds are being eliminated** because of annealing. We are awaiting further results from two-level system calculations
- Preliminary results from vapor deposition simulations of *α*-Si show that **we can model the dependence of mechanical loss on substrate temperature**.
- More works are being done to **translate this knowledge into predicting the unknown**: better dopants, ideal substrate temperature *etc.*

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