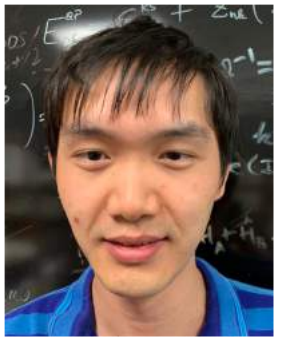
Current Progress on Atomistic Modeling and Simulation of Coating Materials

Hai-Ping Cheng[1]
Jun Jiang[1], Alec S. Mishkin[1], Rui Zhang[1],
Kiran Prasai[2], Riccardo Bassiri[2], Martin M. Fejer[2]

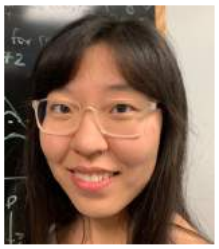
1. Department of Physics and the Quantum Theory Project, University of Florida
2. E. L. Ginzton Laboratory, Stanford University



Jun Jiang

Acknowledgement:

Alec Mishkin

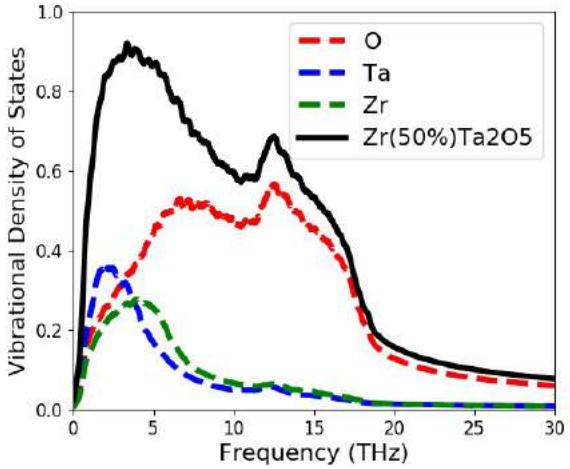


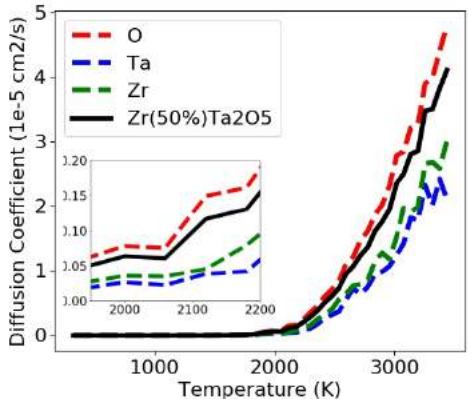
Rui Zhang

Research Highlights

Zhang: Doped Ta_2O_5

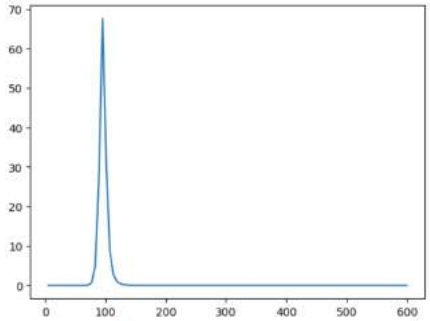
Vibrational DOS 300 K

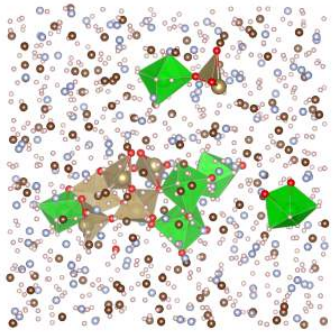




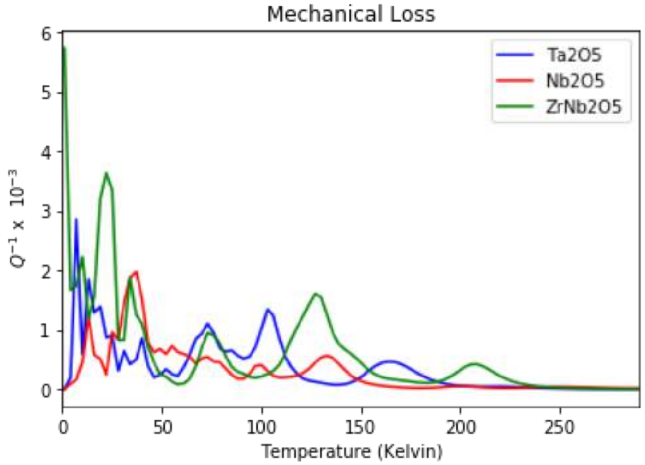
Jun Jiang

A thorough analysis of two-level system in 50% Zr-doped Ta_2O_5 relating loss to atom displacement and much more!



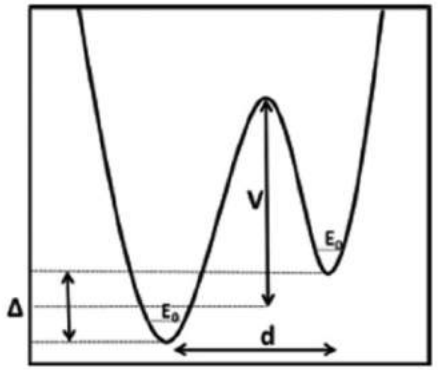


Mishkin: Comparison Ta_2O_5, Nb_2O_5, and 14% Zr doped Nb_2O_5



Zhang: Calculation of Raman spectra is on-going…..

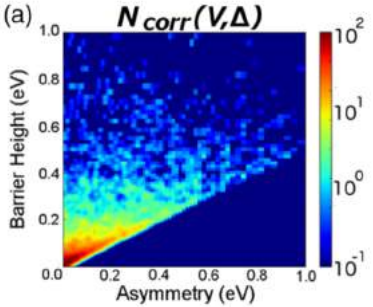
Key parameters for characterizing a TLS: barrier, asymmetry, tau, elastic modulus, coupling constant …



$$Q^{-1}(T) = \frac{1}{3k_bT}\int \frac{\gamma^2\Delta^2}{\epsilon E^2}\frac{\omega\tau}{1+\omega^2\tau^2}\mathrm{sech}^2\left(\frac{E}{2k_bT}\right)n(V,\Delta,\gamma,\tau,\epsilon)dVd\Delta d\gamma d\tau d\epsilon$$

$$\Delta = abs(E_1 - E_2) \qquad E = \sqrt{\Delta^2 + \Delta_0^2}$$

$$V = \frac{V_1+V_2}{2} = E_s - \frac{E_1+E_2}{2} \qquad \tau = \tau_0 \cosh^{-1}\left(\frac{\Delta}{2k_bT}\right)e^{\frac{V}{k_bT}}$$

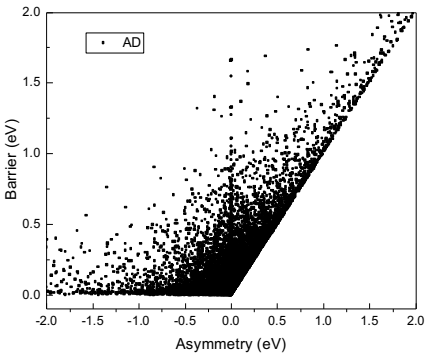


Chris R. Billman, et. al. PRB 95, 014109 (2017)

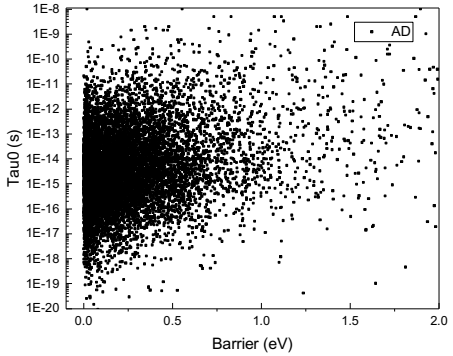
Starting samples: RMC generated to fit expt RDF & DFT relaxed
~40 initial structure for as-deposit and ~40 for annealed (800k)

Parameters distribution (barrier, asymmetry, tau…) for AD and AN 50% ZrO_2 doped Ta_2O_5

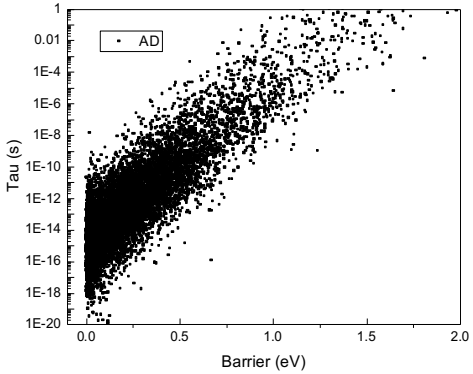
barrier vs asymmetry



barrier vs tau0

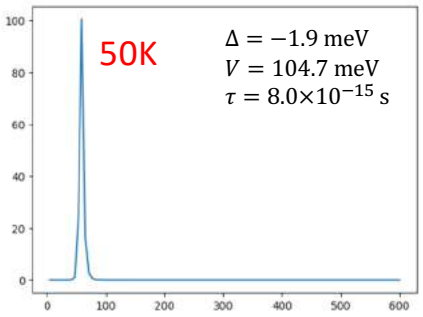


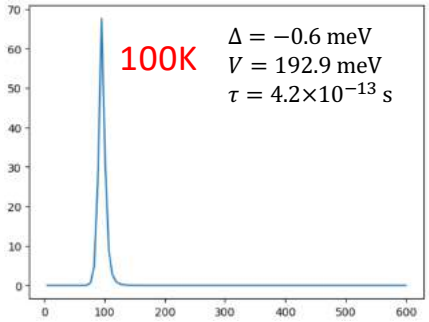
barrier vs tau

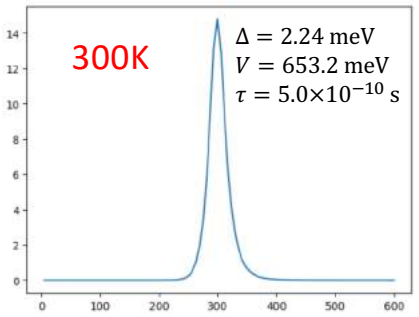


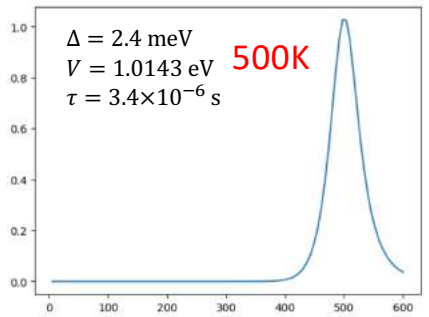
New modifications for a better description of TLS: $\Delta = abs(E_1 - E_2)$ → Δ_1 and Δ_2 $V = \frac{V_1+V_2}{2}$ → V_1 and V_2

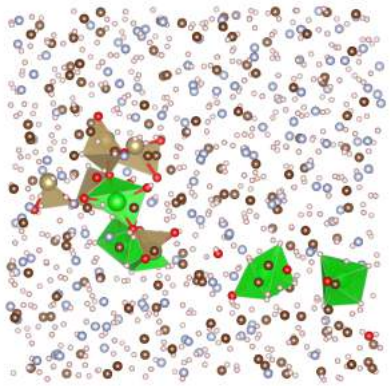
Mechanical Loss from a single transition

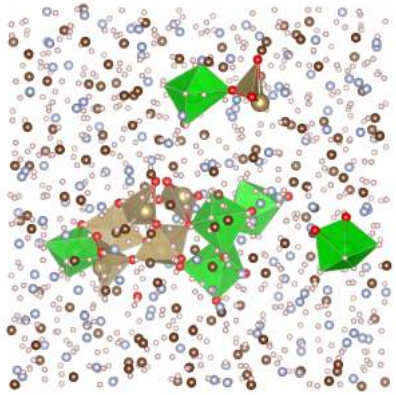


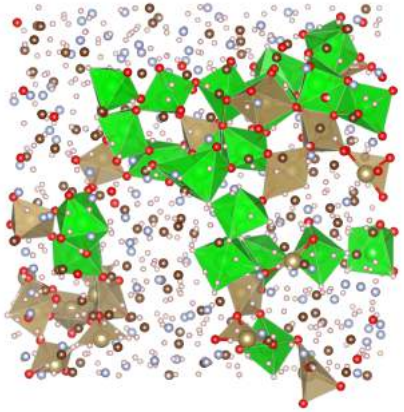




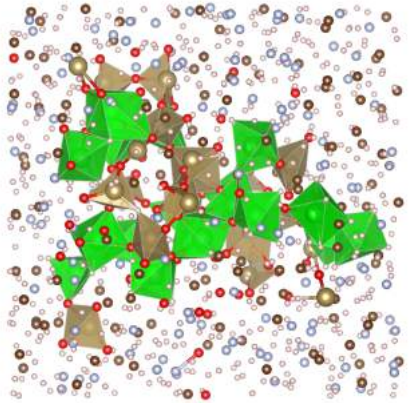








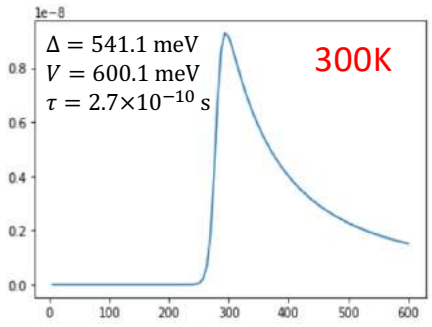
Chain

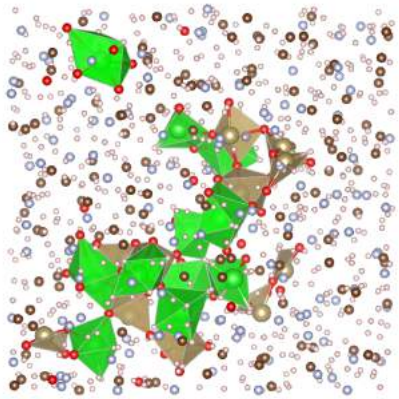


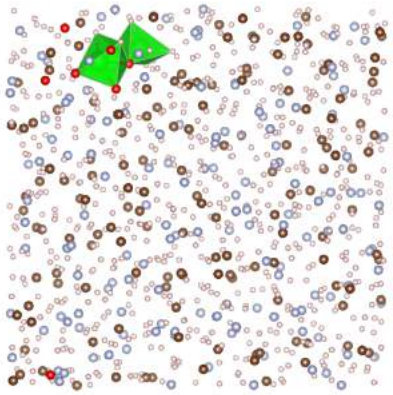
Cluster

Atoms moves more than 0.1 A during transition. Green: Zr and Brown Ta; Oxygens are red dots

Mechanical Loss from a single transition



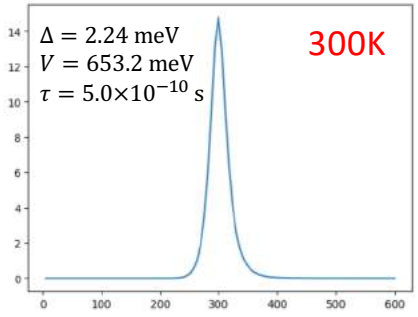


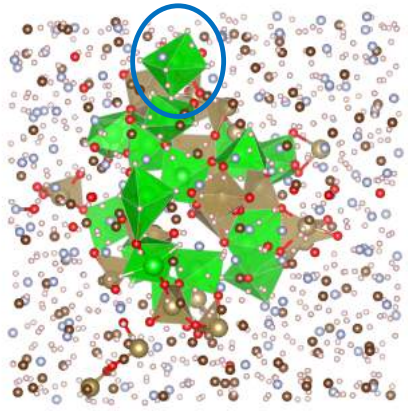


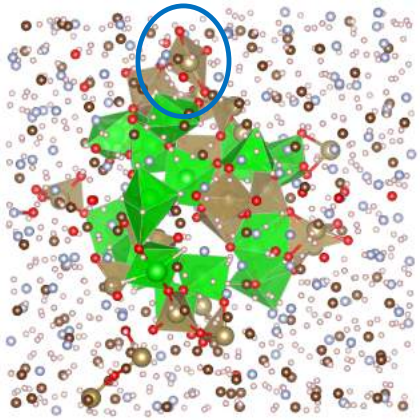
Large Asymmetry

Minimum1 -> Saddle

Saddle -> Minimum2

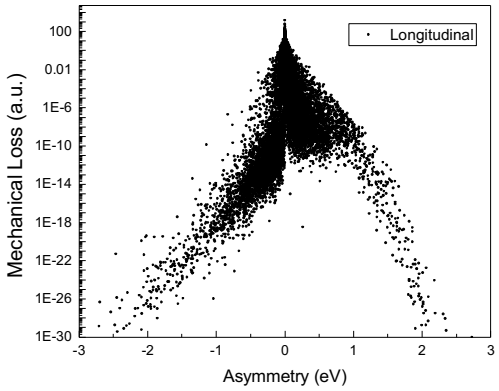


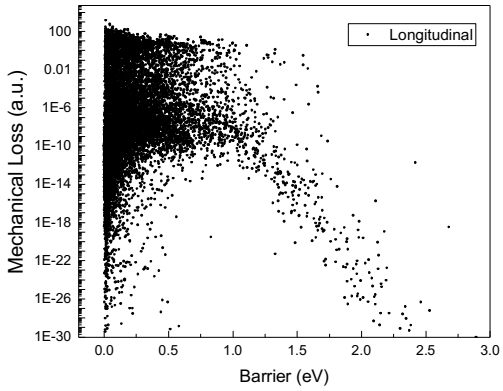


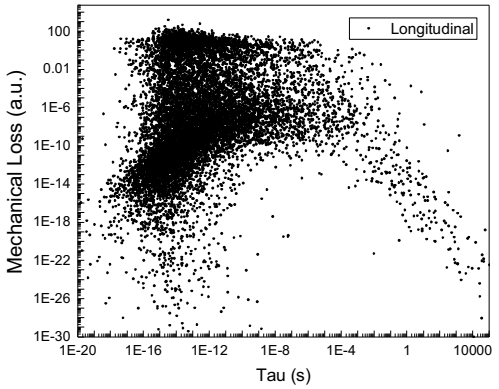


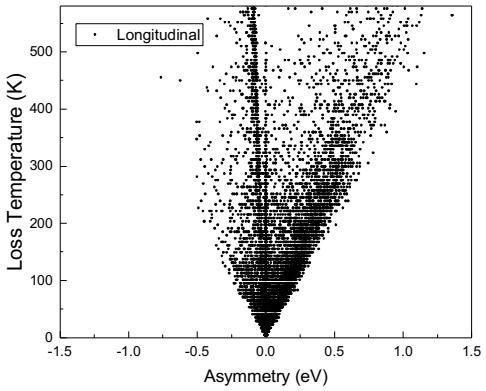
Small Asymmetry

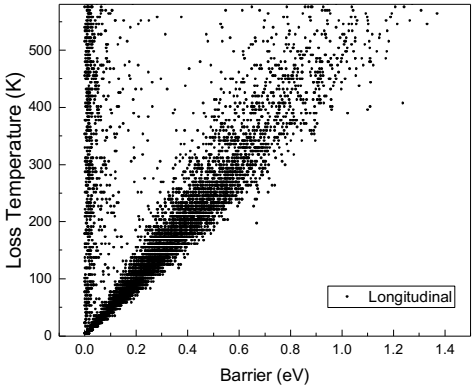
Mechanical Loss vs Barrier (Asymmetry, relaxation time)

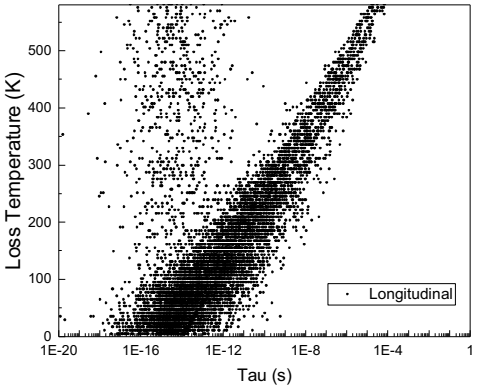








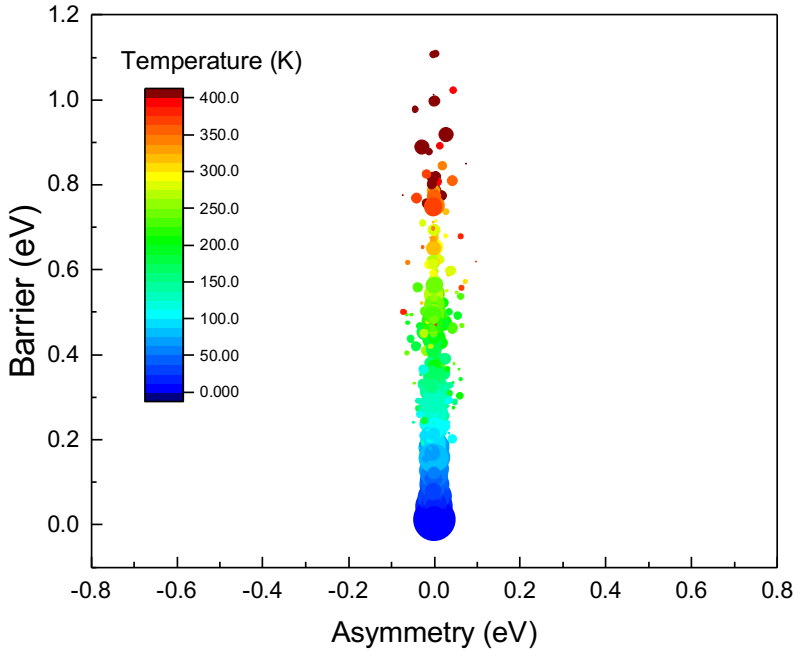


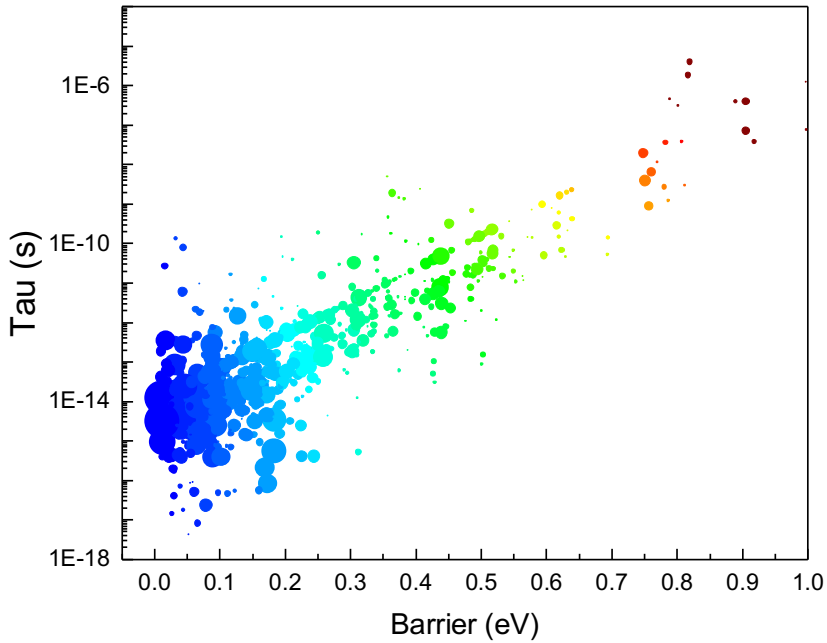


Identify the relation between loss peak centers at different temperature with barrier, asymmetry and relaxation time.

TLSs that has large contribution to mechanical loss

Color: Temperature
Size: Diameter ∝ Log(loss)

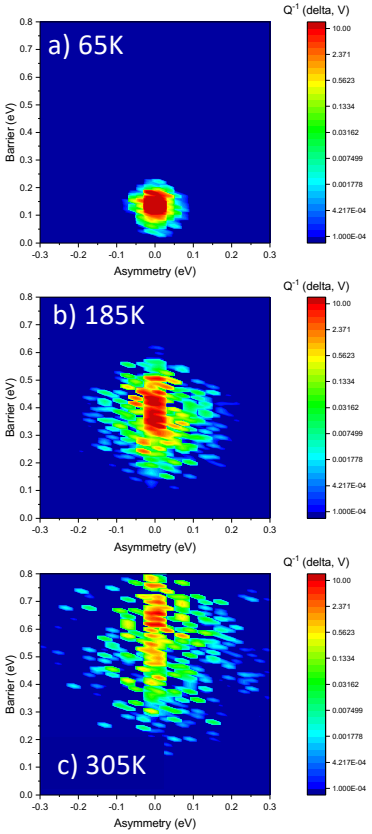


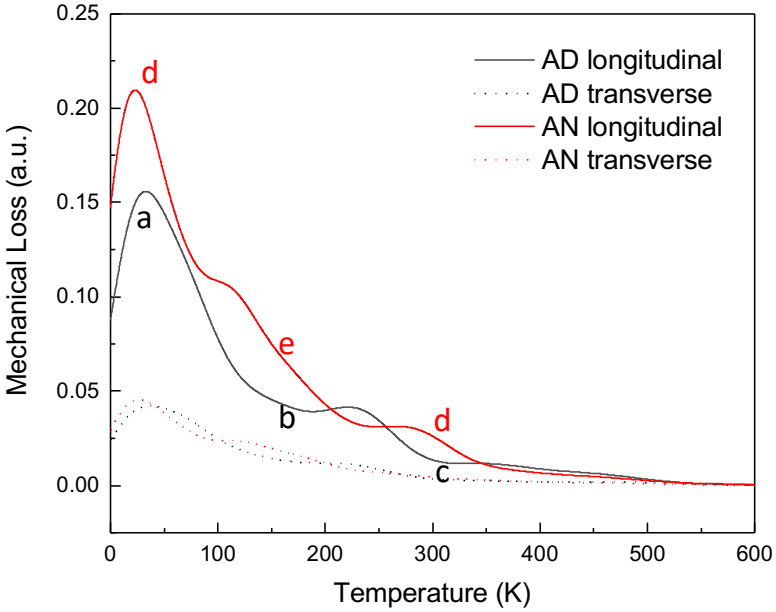


Low asymmetry gives main loss contribution; Higher barrier gives loss at higher temperature

Mechanical Loss of 50% ZrO_2 doped Ta_2O_5

AD

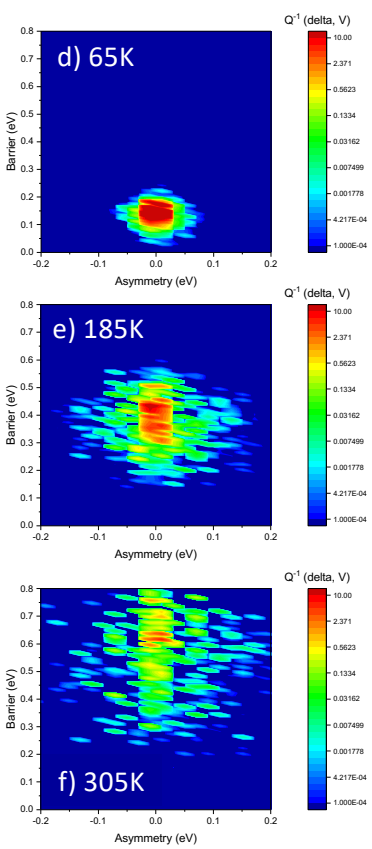




	Large Loss (%)	Large Loss T>200K (%)	Small Loss (%)	Small Loss T>200K (%)
AD	12.30	1.95	87.70	50.40
AN	13.46	1.62	86.54	48.27

TLS number percentage of loss contribution at low (T<200K) or high (T>= 200K) temperature

AN



Calculated transverse loss is smaller than Longitudinal loss.

The AN models have larger mechanical loss compare to AD models, except the range about 240 K.

Summary

- Main mechanical loss is contributed by low asymmetry TLS transition
- TLS transitions with higher barrier give loss at higher temperature
- Calculated mechanical loss for AN (800C annealed) is higher than AD (As-deposited)