Molecular Dynamics simulations to study dissipation in amorphous SiNx

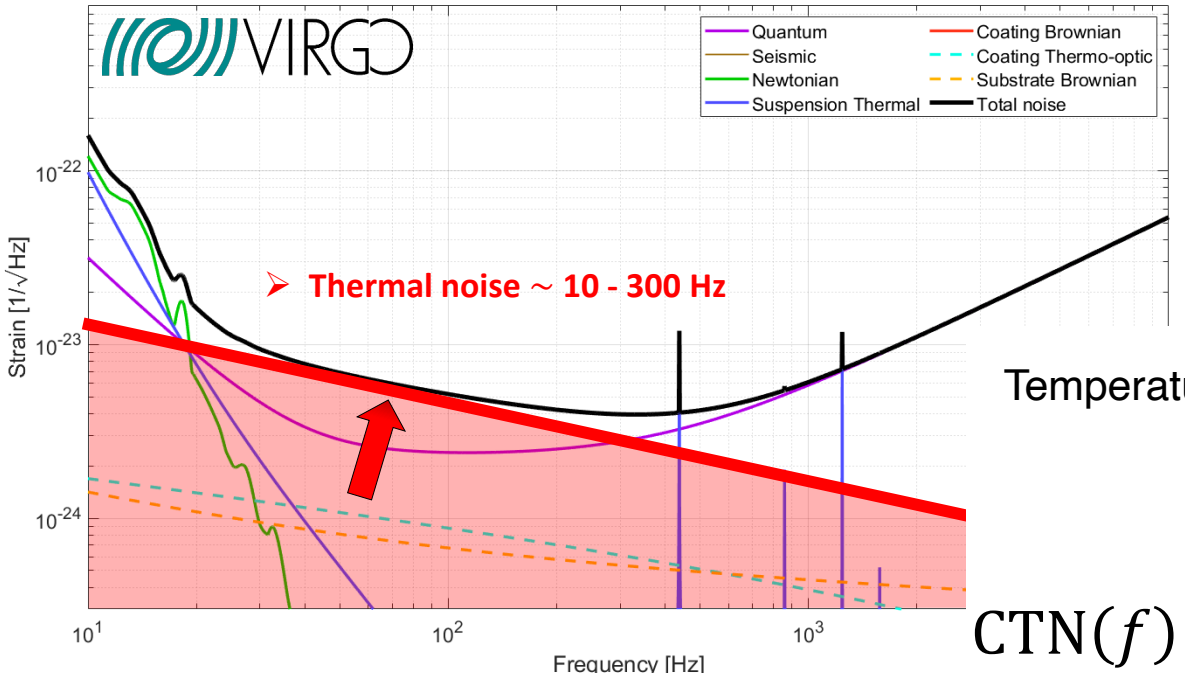
F. Puosi[a], F. Fidecaro[a,b], S. Capaccioli[b], D. Pisignano[b], D. Leporini[b]

[a] INFN Pisa

[b] University of Pisa

Contact: francesco.puosi@pi.infn.it

Coating thermal noise



Coating Thermal Noise (CTN) limits the detection band in the "bucket" (middle frequencies) which is the most sensitive region of the GW detectors.

Temperature

Mechanical loss

$$\mathrm{CTN}(f) \propto \frac{\sqrt{\frac{T}{f}\,\frac{1}{w^2}\,\varphi\, d}}{L}$$

Coating thickness

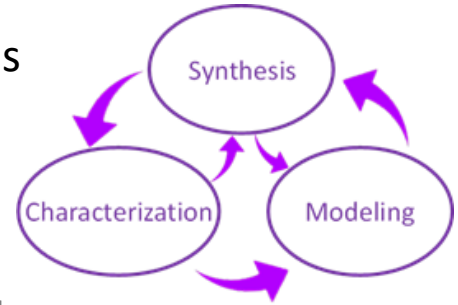
Arm length

Beam-size

VCR&D

Goal: increase the mechanical performances of current coating materials

An intensive, cooperative effort is ongoing within the VCR&D to provide comprehensive characterization of **SiNx**



Atomistic Simulation of SiN

Scrutinizing the existing interatomic potentials for SiN:

- **Tersoff potential**: strong impacts of short cut-offs on the structure
- **Marian-Gastreich 3-body potential**: tendency to over-coordinate atoms
- **Vashisht potential**: tendency to create crystalline structures
- **Garofalini potential**: OK
- **Marian-Gastreich 2-body potential**: OK and computationally efficient

Attractive interaction

$$\mathrm{E_{N-Si}} = \mathrm{Morse} = D_e\left\{1 - e^{-a(r-r_0)^2} - 1\right\}$$

Screened Coulomb repulsion

$$\mathrm{E_{N-N/Si-Si}} = \mathrm{General} = \frac{A}{r}e^{-r/\rho}$$

$$\mathrm{E_{N-N}} = -\frac{C_6}{r^6}\left(1 - e^{-b_6 r}\sum_{k=0}^{6}\frac{(b_6 r)^k}{k!}\right)$$

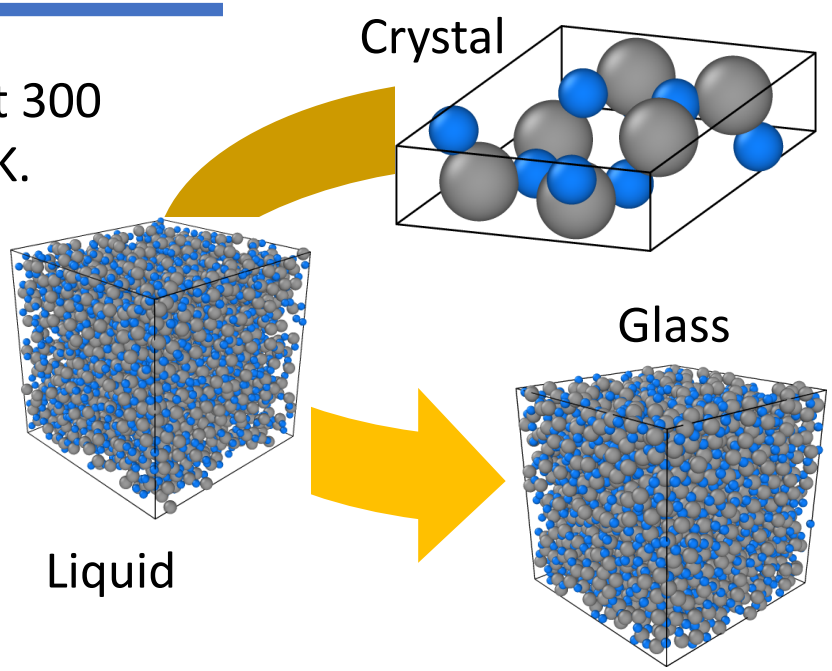
Dispersion interaction

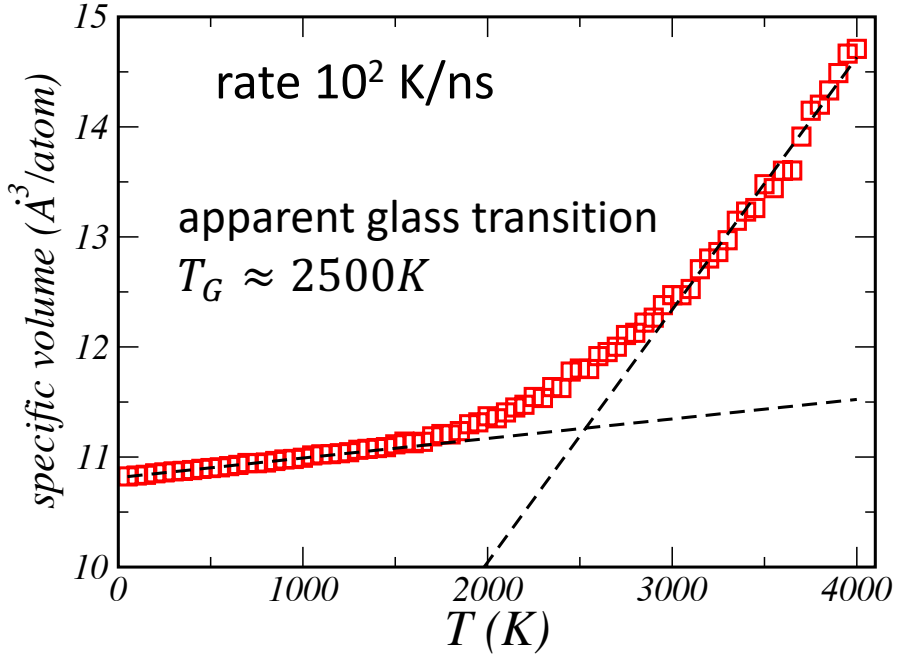
Phys. Rev. B 62 (2000) 3117

Amorphous Si_3N_4

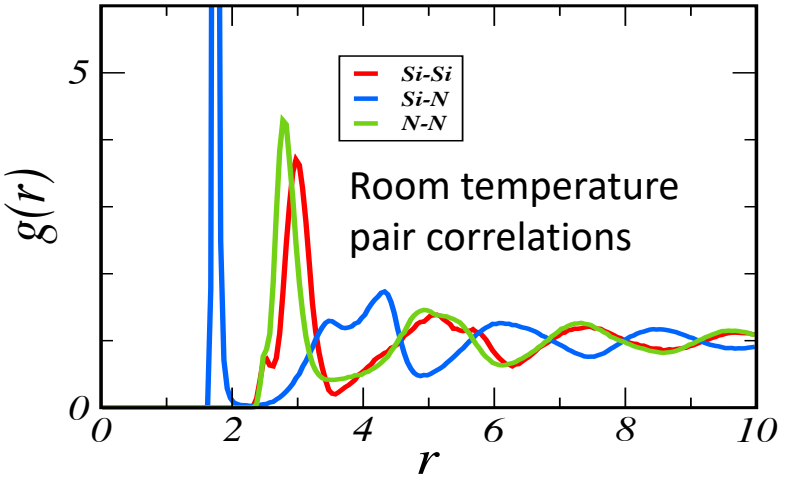
Liquid samples: start from crystal (β-phase) at 300 K, fast heating to 5000 K, equilibrate at 5000 K.

Glasses by cooling the liquid at constant rate.

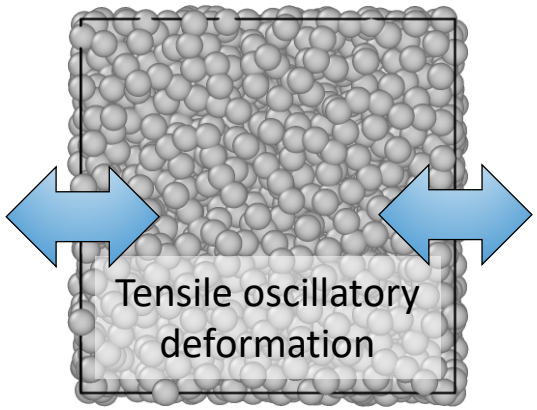




Clear evidence of amorphous structure



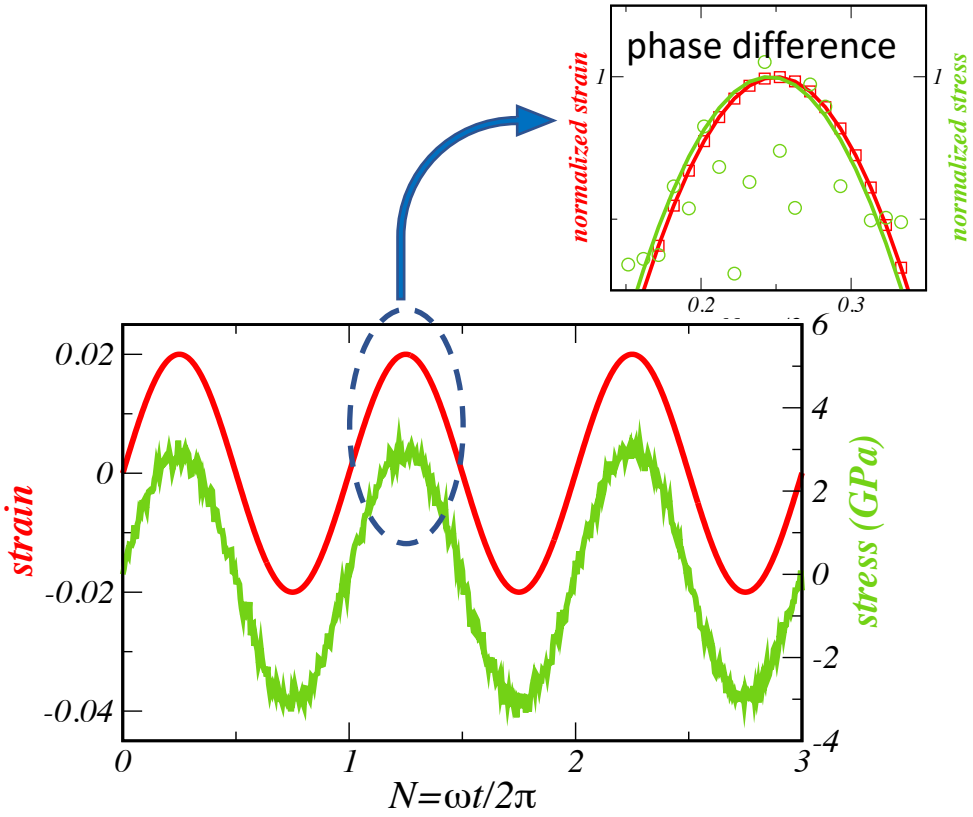
Dynamical mechanical spectroscopy



Apply a numerical strain and compute the corresponding stress

Mechanical losses are estimated from the phase shift

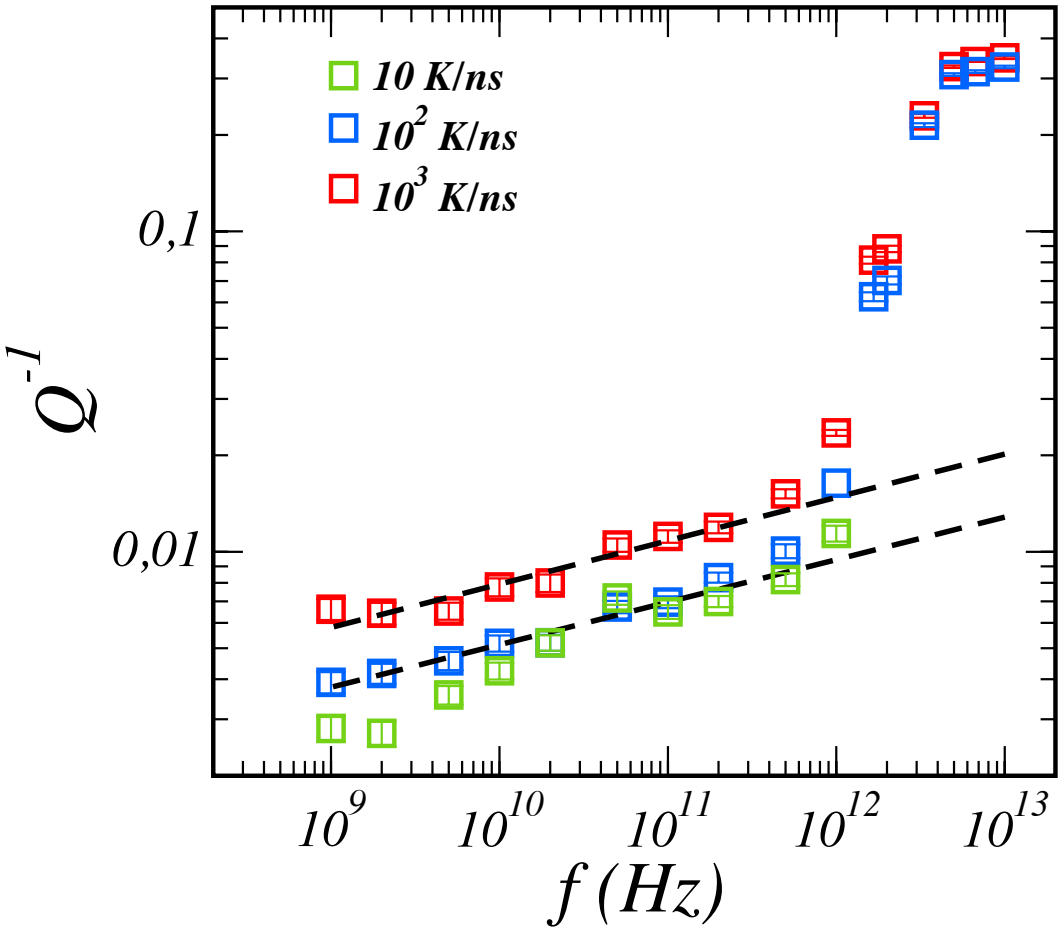
$$Q^{-1} = \tan\delta = \frac{E''}{E'}$$



Previous works based on this approach have reported remarkable agreement between simulation results and experimental data on on Ta_2O_5.

(Phys. Rev. Research **1** 033121 (2019), Acta Materialia **201** 1 (2020))

Mechanical losses in Si_3N_4



Dissipation dues to Rayleigh scattering at very high frequency (observed in several amorphous materials but missing in other high coordination number glasses like SiC).

Apparent power-law behavior in the GHz range with exponent $n \sim 0.13$, similar to what reported for Ta_2O_5.

A slower quench from the liquid phase results in glasses with reduced dissipation. Yet, this cooling rate effect is not strong.

Conclusions and perspectives

In the simulation range of frequency, dissipation in Si3N4 exhibits a behavior similar to what observed in oxide glasses (Rayleigh scattering, power-law dependence on *f*).

For the slowest quenched glasses, losses are reduced with respect to Ta_2O_5 by a factor 2.

Extrapolating to experimentally relevant frequencies (1 KHz) results in $\boldsymbol{Q^{-1} \approx 5\times10^{-4}}$, which compares well with the experimental values measured in deposited Si_3N_4.

Next steps:

Microscopic characterization of the dissipation phenomenon.

Modeling of different sample preparation methods (deposition?)