Gravitational Wave Advanced Detector Workshop 2021

Molecular Dynamics simulations to study dissipation in amorphous SiNx

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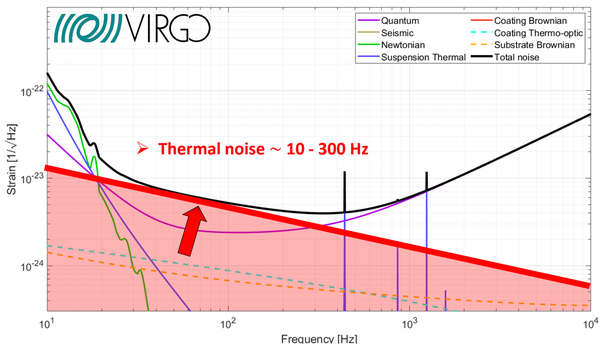
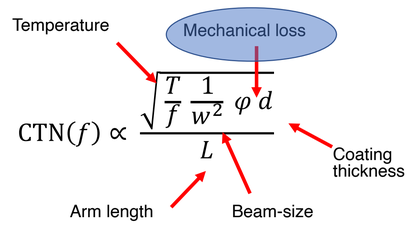
1. Coating thermal noise

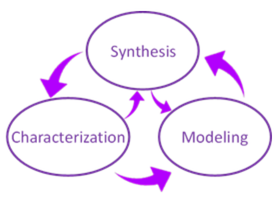


Coating Thermal Noise (CTN) limits the detection band in the "bucket" (middle frequencies) which is the most sensitive region of the GW detectors.



Goal: increase the mechanical performances of current coating materials.

An intensive, cooperative effort is ongoing within the VCR&D to provide comprehensive characterization of **silicon nitride SiNx** which represents a promising candidate as a possible solution for the reduction of mechanical losses in coating films.



Simulations and modeling are standard tools for studying glasses and can be of help in the material selection by providing a "quick" estimate of mechanical losses.

2. Atomistic simulation of SiNx

Scrutinizing the existing interatomic potentials for classical Molecular Dynamics simulations of 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

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

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

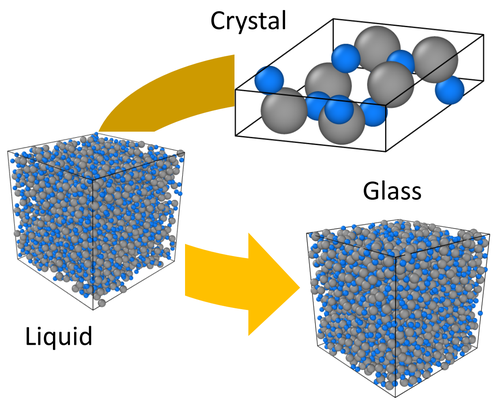
Dispersion interaction

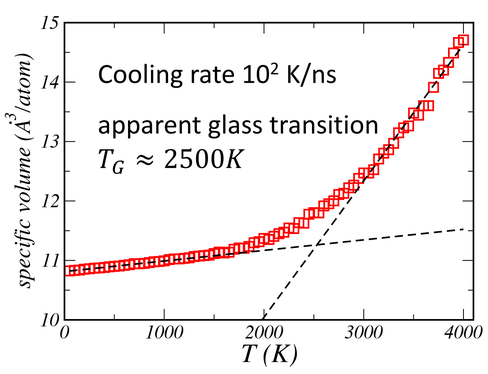
Phys. Rev. B 62 (2000) 3117

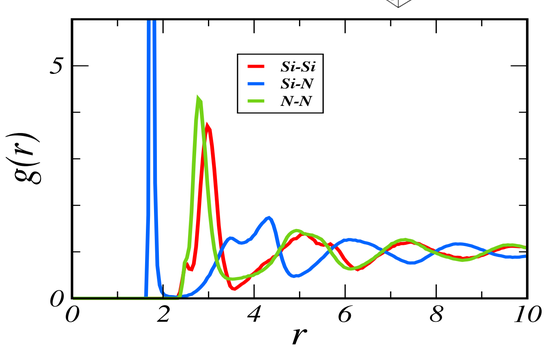
3. Amorphous Si_3N_4

Glasses by melt quenching:

Crystalline Si_3N_4 is first equilibrated at 300K and then rapidly heated to 5000K.
The liquid at 5000K is equilibrated and then cooled down to 300K at constant rate in the NPT ensemble (zero pressure).

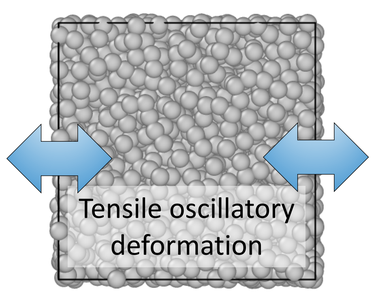






Pair correlation function *g(r)* indicate an amorphous structure.

4. Simulated Dynamical Mechanical Spectroscopy

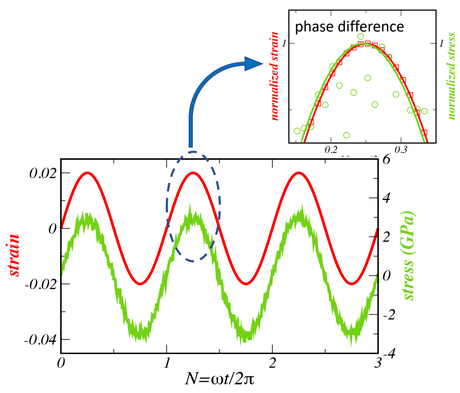


Dynamical Mechanical Spectroscopy (DMS) was performed by imposing to the simulation box a sinusoidal tensile strain $\varepsilon_{ii}(t) = \varepsilon_0 \sin(\omega t)$ in the *i*-direction ($i = X, Y$ or Z), and measuring the corresponding tensile stress along the same direction, σ_{ii}. The results were averaged over all the three directions, and the frequency $f = \omega/2\pi$ was varied from 0.5 GHz to 1 THz. We fixed the amplitude $\varepsilon_0 = 0.01$, such that the deformation is in the linear elastic regime. A thermostat was employed to maintain constant temperature conditions and dissipate the heat produced during the deformation.

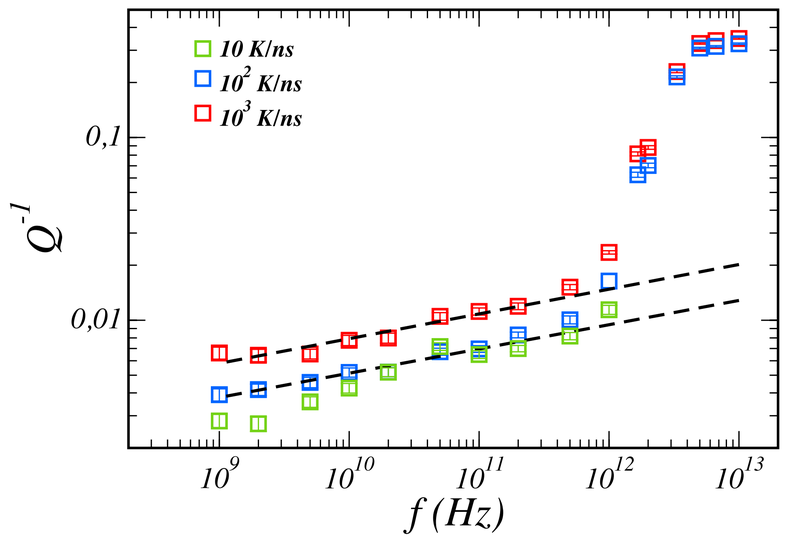
Mechanical losses, i.e. the quality factor, are estimated from the stress-strain phase difference:

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

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))



5. Results of mechanical losses in Si_3N_4



Dissipation controlled by Rayleigh scattering at very high frequency. This behavior was observed in several amorphous materials but missing in other high coordination number glasses like SiC.

Apparent power-law behavior in the GHz range with an exponent $n \sim 0.13$, similar to the value 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.

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

6. Conclusions and perspectives

In the simulation range of frequency, dissipation in Si_3N_4 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.

Via an extrapolation we estimate a value for mechanical losses at experimentally relevant frequencies which is in good agreement with the experimental values measured in deposited Si_3N_4.

Next steps:

A microscopic characterization of the dissipation phenomenon.

Modeling of different sample preparation methods which "resemble" the experimental ones (deposition?)

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