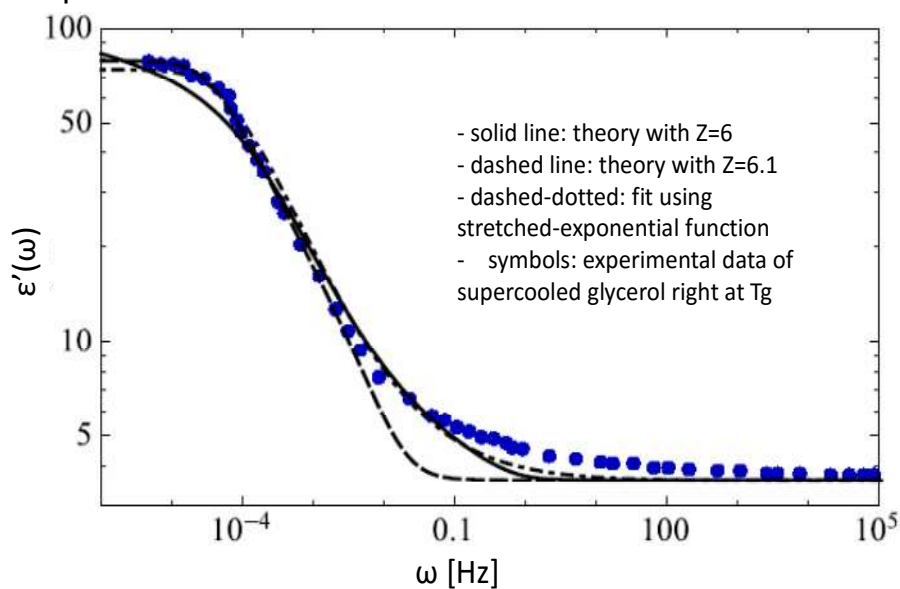


# Microscopic theory of dielectric and mechanical response of disordered materials

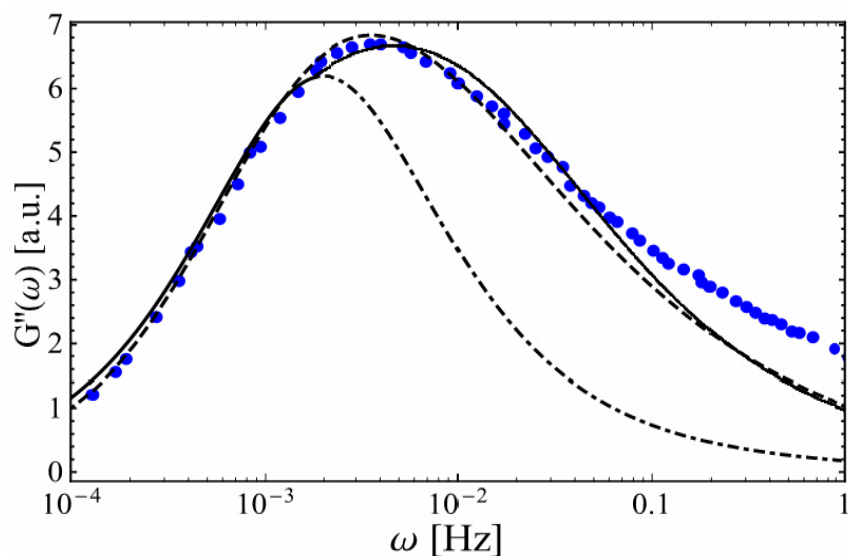
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## Project Description

The intern works with the theoretical framework developed in the Statistical Physics Group at the Department of Chemical Engineering and Biotechnology to predict the dielectric and mechanical response of organic and metallic glasses from the calculation of the vibrational modes [1]. The framework uses sum rules for the dielectric and mechanical response that account for the disordered spatial distribution of the microscopic building blocks. The final outcome in terms of dielectric relaxation and shear modulus function will be analysed for different models and used to fit experimental data recorded at glass transition temperature that corresponds to coordination number  $z \approx 6$ . The various models of non-Markovian friction will be compared both in terms of their performance in the fitting of experimental data.



Comparison in dielectric constant between our theory and the experimental data of glycerol from Ref. [2].



Comparison of dissipative part of shear modulus between our theory and the experimental data of metallic glasses from Ref. [3].

## Project Impact

The possibility of predicting yielding and mechanical energy-absorption of amorphous materials at the atomic/molecular scales will open new possibilities for material modelling in aircraft and aerospace engineering. Using the new theory, we will come up with chemical design principles to optimize energy absorption upon impact (e.g. by changing the monomer mixture, the crosslinking etc.) and this idea will lead to new materials able to save human lives in accidents, blasts or in war context.

## References:

- [1] R. Milkus and A. Zaccone, Phys. Rev. B (2016).
- [2] P. Lunkenheimer, U. Schneider, R. Brand and A. Loid, Contemporary Phys. 41, 1 (2000).
- [3] J. M. Pelletier, J. Alloys Compd. 393, 223 (2005).

## Main Text

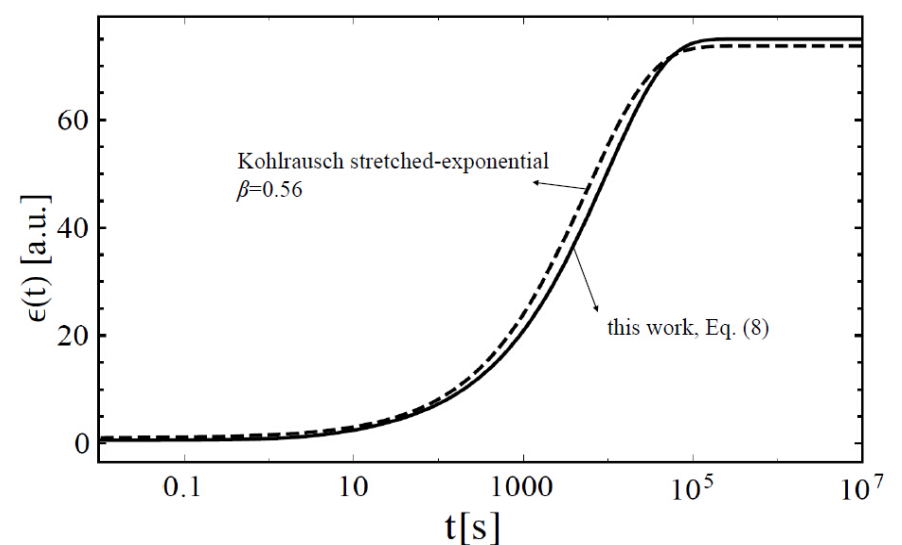
In a disordered solid, a tagged molecule is not a local center of inversion symmetry, and it strongly interacts with other molecules. The forces transmitted to it by its nearest-neighbours, which are also being molecule. This non-zero force generates an additional nonaffine displacement. The lattice dynamics of dielectric response to account for this critical effect due to disorder can be generalized for dielectric relaxation and mechanical shear modulus which involve the vibrational density of states and well-known boson peak anomaly at low eigenfrequencies. The theory describes the asymmetric  $\alpha$ -relaxation of the loss modulus, which cannot be predicted without accounting for both nonaffinity and the boson peak.

In dielectric relaxation, the permittivity can be expressed as a function of either external frequency of applied field or time, which are

$$\epsilon^*(\omega) = 1 - \int_0^{\omega_D} \frac{A\rho(\omega_p)}{\omega^2 - i(\nu/m)\omega - C^2\omega_p^2} d\omega_p$$

$$\epsilon(t) = B + \int_0^{\omega_D} \frac{AD(\omega_p)}{2K} \left( \frac{e^{(K-\frac{\nu}{2m})t}}{K - \nu/2m} + \frac{e^{-(K+\frac{\nu}{2})t}}{K + \nu/2m} \right) d\omega_p$$

$$K \equiv \sqrt{(C\omega_p)^2 - \frac{\nu^2}{4m^2}}$$



Comparison of dielectric relaxation between our theory and stretched exponential function.

Likewise, we also write viscoelastic shear modulus in either frequency or time domain:

$$G(\omega) = G^{Born} + \frac{3\rho}{m} \int_0^{\omega_D} \frac{D(\omega_p)\Gamma(\omega_p)}{\omega^2 - i(\tilde{\nu}(\omega)/m)\omega - C^2\omega_p^2} d\omega_p$$

$$G(t) = G^{Born} - \frac{3\rho}{m} \left[ \Theta(t) * H(t) - \sum_n \Gamma(\omega_p) \frac{\pi}{c^2\omega_p^2} \right]$$