Modeling viscoelasticity and energy dissipation in Silica in the THz regime

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Abstract

The attenuation of sound waves in glasses is still poorly understood, partly because the underlying mechanism strongly depends on the frequency of the incident wave and on the ratio between its wavelength and the characteristic length scales of the glasses. Here, we investigate energy dissipation in oxide glasses using atomic-scale simulations. We employ Molecular Dynamics (MD) to measure energy dissipation using simulated mechanical spectroscopy in the GHz and THz regimes in a model SiO2 glass. We find that the computed dissipation compares favorably with existing experimental data. We also show that when the forcing frequency lies within the frequency range of the main band of normal modes of the system, dissipation is harmonic. We develop an exact analytical expression of the energy dissipation in the harmonic approximation, which allows to study the contribution of individual vibration modes to the overall dissipation. We show that dissipation arises mainly from the non-affine bending of Si-O-Si bonds triggered by the applied affine deformation. Moreover, this expression, valid both below and above the Ioffe-Regel (IR) crossover, extends the domain of application of the usual treatment of sound attenuation in glasses based on fitting the dynamical structure factor with damped harmonic oscillators, which is valid only bellow the IR limit.

Reference:

Damart T., Tanguy A., Rodney D. 'Theory of harmonic dissipation in glasses' *Physical Review B* **95** (2017) 054203.

Keywords: energy dissipation, atomistic modeling, harmonic dynamics

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