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Molecular Dynamics simulations to study dissipation in amorphous materials: starting with Ta_2O_5

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In interferometric gravitational wave detectors, thermal noise from the mirrors represents currently the major limitation in most of the detection band. It originates from mechanical dissipation, which is rather low in the substrates, but orders of magnitude higher in the coating films. Although a significant experimental effort has led to some improvements during these years, there is still a lack of fundamental understanding of the involved dissipation mechanisms, which is critically limiting the development of effective design tools for successful coating architectures. The common approach to this problem builds on the framework of the so-called two-level systems (TLS) model [1]: dissipation is due to the atomic motion originating from a transition between two potential energy minima, promoted by the coupling between thermal activation and mechanical waves. In the last decades, the TLS model has been used to fix experimental data or to predict dissipation via atomic scale simulations, paying the price of simplifying approximations and heavy computations. In this work we propose a different numerical approach to study dissipation in glasses, which, in contrast to TLS, is theory-independent as it does not require any a priori assumption [2]. We apply the experimental protocol of the mechanical spectroscopy to atomistic simulations, in which a glass is subjected to oscillatory deformation at a given frequency f and the storage and loss moduli are measured. We test the method on glassy Ta_2O_5, created by melt cooling. We find that in the GHz range the quality factor follows a robust power-law dependence on f, whose specific form depends on temperature and thermal history. Further, after an extrapolating to the kHz range of interest, simulation results exhibit strong qualitative and satisfying quantitative agreement with the existing experimental data. Our results suggest that in silico mechanical spectroscopy has the potential to push the predictive power down to millisecond timescale in amorphous coatings.

References:
[1] W.A. Phillips, J. Low. Temp. Phys. 7, 351 (1972).
[2] F. Puosi, F. Fidecaro, S. Capaccioli, D. Pisignano and D. Leporini, in preparation.

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