
Atomistic study of two-level systems in amorphous silica

Tanguy Damart¹ and David Rodney*¹

¹Institut Lumière Matière (ILM) – CNRS : UMR5306, Université Claude Bernard - Lyon I (UCBL) – UMR5306 CNRS Université Claude Bernard Lyon 1 Domaine Scientifique de La Doua Bâtiment Kastler, 10 rue Ada Byron 69622 Villeurbanne CEDEX, Franc, France

Abstract

We model at the atomic-scale internal friction in amorphous silica at low frequencies. To this aim, we explore the potential energy landscape of multiple glass samples to identify two-level systems (TLSs). We discuss the properties of TLSs, particularly their energy asymmetry and barrier as well as their deformation potential, computed as longitudinal and transverse averages of the full deformation potential tensors. The discrete sampling is used to predict dissipation in the classical regime. Comparison with experimental data shows a better agreement with poorly relaxed thin films than well relaxed vitreous silica, as expected from the large quench rates used to produce numerical glasses. The TLSs are categorized in three types that are shown to affect dissipation in different temperature ranges. The sampling is also used to discuss critically the usual approximations employed in the literature to represent the statistical properties of TLSs.

Reference:

T. Damart, D. Rodney, 'Atomistic study of two-level systems in amorphous silica ', Physical Review B 97, 014201 (2018).

Keywords: internal friction, atomistic modeling

*Speaker