

## Collective dynamics in a glass: a molecular dynamics study

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Collective excitations in glasses are very interesting phenomena which were extensively studied lately. The reason for that was presence of excess low-frequency excitations which give rise to boson peak in density of vibrational states. The nature of both is still unknown. The goal of our investigation was to shed light on this problem and to look at it from a new point of view.

We have carried out molecular dynamics simulations of two Lennard-Jones binary glasses: the Wahnström [1] and Kob-Andersen [2] models. Total and concentration autocorrelation functions were calculated for collective density and current. Their fourier transforms were used to find the vibrational modes frequency for different wavenumbers, thus giving dispersion curves.

We have also investigated the motions of atoms, and it turned out that they can be separated into two distinct types which move differently: active, jumping between equilibrium sites, and static, vibrating around single equilibrium point. We have found strong connection between excess low-frequency modes and movement of the active atoms. The dynamics of separate atom jumps between equilibrium sites was studied as well.

[1] T. Schröder, S. Sastry, J. Dyre and S. Glotzer, *J. Chem. Phys.*, 2000, **112**, 9834.

[2] W. Kob and H. Andersen, *PRL*, 1994, **73**, 1376.