Acoustic properties in glycerol glass-former: Molecular dynamics simulation

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TUT DES MATERIAUX ET MOLECULES DU MANS TEAM — Study of high-
frequency collective dynamics around TeraHertz region in glass former has been a
subject of intense investigations and debates over the past decade. In particular,
the presence of the Boson peak characteristic of glassy material and its relation to
other glass anomalies. Recently, experiments and simulations have underlined possi-
ble relation between Boson peak and transverse acoustic modes in glassy materials.
In particular, simulations of simple Lennard Jones glass former have shown a rela-
tion between Ioffe-Regel criterion in transverse modes and Boson peak. We present
here molecular dynamics simulation on high frequency dynamics of glycerol. In or-
der to study mesoscopic order (0.5-5nm$^{-1}$), we made use of large simulation box
containing 80000 atoms. Analysis of collective longitudinal and transverse acoustic
modes shows striking similarities in comparison with simulation of Lennard-Jones
particles. In particular, it seems that a connection may exist between Ioffe-Regel
criterion for transverse modes and Bose Peak frequency. However, in our case we
show that this connection may be related with structural correlation arising from
molecular clusters.

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