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Acoustic properties in glycerol glass-former: Molecular dynamics simulation REMI BUSSELEZ, THOMAS PEZERIL, Universite du Maine, INSTITUT 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 possible relation between Boson peak and transverse acoustic modes in glassy materials. In particular, simulations of simple Lennard Jones glass former have shown a relation between Ioffe-Regel criterion in transverse modes and Boson peak. We present here molecular dynamics simulation on high frequency dynamics of glycerol. In order to study mesoscopic order ($0.5\text{-}5\text{nm}^{-1}$), 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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