



How do packing defects modify the cooperative motions in supercooled liquids?

Submitted by Victor Teboul on Mon, 05/01/2017 - 21:52

Titre	How do packing defects modify the cooperative motions in supercooled liquids?
Type de publication	Article de revue
Auteur	Taamalli, Sonia [1], Belmabrouk, Hafed [2], Van Hoang, Vo [3], Teboul, Victor [4]
Pays	Pays-Bas
Editeur	Elsevier
Ville	Amsterdam
Type	Article scientifique dans une revue à comité de lecture
Année	2017
Langue	Anglais
Date	20 Juin 2017
Pagination	55-61
Volume	490
Titre de la revue	Chemical Physics
ISSN	0301-0104
Mots-clés	Dynamic heterogeneity [5], Glass-transition [6]
Résumé en anglais	<p>We use molecular dynamic simulations to investigate the relation between the presence of packing defects in a glass-former and the spontaneous cooperative motions called dynamic heterogeneity. For that purpose we use a simple diatomic glass-former and add a small number of larger or smaller diatomic probes. The diluted probes modify locally the packing, inducing structural defects in the liquid, while we find that the number of defects is small enough not to disturb the average structure. We find that a small packing modification around a few molecules can deeply influence the dynamics of the whole liquid, when supercooled. When we use small probe molecules, the dynamics accelerates and the dynamic heterogeneity decreases. In contrast, for large probes the dynamics slows down and the dynamic heterogeneity increases. The induced heterogeneities and transport coefficient modification increase when the temperature decreases and disappear around the onset temperature of the cage dynamics.</p>
URL de la notice	http://okina.univ-angers.fr/publications/ua15896 [7]
DOI	10.1016/j.chemphys.2017.04.006 [8]
Lien vers le document	https://authors.elsevier.com/a/1Uw1L_6s1nvv90 [9]

Liens

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[2] <http://okina.univ-angers.fr/publications?f%5Bauthor%5D=25562>

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