Cooperative motions in a finite size model of liquid silica: an anomalous behavior

Submitted by Victor Teboul on Wed, 03/04/2015 - 17:55

Titre	Cooperative motions in a finite size model of liquid silica: an anomalous behavior
Type de publication	Article de revue
Auteur	Teboul, Victor [1]
Editeur	EDP Sciences
Type	Article scientifique dans une revue à comité de lecture
Année	2006
Langue	Anglais
Date	2006-05-01
Numéro	1
Pagination	111-118
Volume	51
Titre de la revue	European Physical Journal B: Condensed Matter and Complex Systems
ISSN	1434-6028

Résumé en anglais	Finite size effects on dynamical heterogeneity are studied in liquid silica with Molecular Dynamics simulations using the BKS potential model. When the system size decreases relaxation times are found to increase in accordance with previous results in finite-size simulations and confined liquids. It has been suggested that this increase may be related to a modification of the spatially heterogeneous dynamics in confined liquids. In agreement with this hypothesis we observe a decrease of the spatially heterogeneous dynamics when the size decreases. The spatially heterogeneous dynamics is usually characterized by the dynamical aggregation of the most or the least mobile atoms. However we find that the decrease of the dynamical aggregation associated to the least mobile atoms is much more important than the decrease associated to the most mobile atoms when the size decreases. This result associated with a slowing down of the liquid is surprising as it is expected that the dynamical aggregation of the least mobile atoms should increase the slowing down of the liquid dynamics. The decrease of the heterogeneous behaviour is also in contradiction with the increase of the spatially heterogeneous dynamics observed in liquids confined inside nanopores. However, an increase of the non-Gaussian parameter appears both for the confinement inside nanopores and for the finite size simulations. As the non-Gaussian parameter is usually associated with the heterogeneous dynamics, the increase of the non-Gaussian parameter together with a decrease of the spatially heterogeneous dynamics is also surprising.

URL de la notice	http://okina.univ-angers.fr/publications/ua8567 [2]
DOI	10.1140/epjb/e2006-00186-9 [3]

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[3] http://dx.doi.org/10.1140/epjb/e2006-00186-9