Enhanced diffusion in finite-size simulations of a fragile diatomic glass former

Titre	Enhanced diffusion in finite-size simulations of a fragile diatomic glass former
Type de publication	Article de revue
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Pays	Etats-Unis
Editeur	American Physical Society
Ville	College Park
Type	Article scientifique dans une revue à comité de lecture
Année	2016
Langue	Anglais
Date	14 Novembre 2016
Numéro	5
Pagination	052604
Volume	94
Titre de la revue	Physical Review E
ISSN	2470-0045
Résumé en anglais	Using molecular dynamics simulations we investigate the finite-size dependence of the dynamical properties of a diatomic supercooled liquid. The simplicity of the molecule permits us to access the microsecond time scale. We find that the relaxation time decreases simultaneously with the strength of cooperative motions when the size of the system decreases. While the decrease of the cooperative motions is in agreement with previous studies, the decrease of the relaxation time opposes what has been reported to date in monatomic glass formers and in silica. This result suggests the presence of different competing physical mechanisms in the relaxation process. For very small box sizes the relaxation times behavior reverses itself and increases strongly when the box size decreases, thus leading to a nonmonotonic behavior. This result is in qualitative agreement with defect and facilitation theories.
URL de la notice	http://okina.univ-angers.fr/publications/ua15182 [5]
DOI	10.1103/PhysRevE.94.052604 [6]
Lien vers le document	http://journals.aps.org/pre/abstract/10.1103/PhysRevE.94.052604 [7]

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[5] http://okina.univ-angers.fr/publications/ua15182
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