Finite Size Effects and Cooperativity in a Model Diatomic Supercooled Liquid

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Résumé en anglais	We use large scale molecular dynamics simulations to investigate the relation between cooperativity and size e ects in a simple diatomic supercooled liquid. We nd that below a characteristic temperature the transport properties depend on the size of the simulation box. is e ect then increases upon decreasing the temperature. For the model molecules constituting our liquid, the smaller box corresponds to the larger di usion coe cient. us, the size e ects increase the di usion of the liquid with our molecules in opposition with previous results concerning silica and atomic so molecules. As a result, the temperature dependence of the di usion coe cient tends to an Arrhenius law for smaller boxes in our simulations. is result is in agreement with a cooperativity origin of non-Arrhenius behavior and size e ects in fragile supercooled liquids, as a small box cuto cooperative motions thus inducing a constant activation energy. To investigate that picture further we then study the size dependence of cooperative motions in our model liquid.
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