A new scenario of dynamical heterogeneity in supercooled liquid and glassy states of 2D monatomic system

Titre	A new scenario of dynamical heterogeneity in supercooled liquid and glassy states of 2D monatomic system
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Résumé en anglais	Via analysis of spatio-temporal arrangements of atoms based on their dynamics in supercooled liquid and glassy states of 2D monatomic system with a double-well Lennard-Jones-Gauss (LJG) interaction potential, we find a new scenario of dynamical heterogeneity. Atoms with the same or very close mobility have a tendency to aggregate into clusters. Number of atoms with high mobility (and size of their clusters) increases with decreasing temperature passing over a maximum before decreasing downto zero. Position of the peak moves toward a lower temperature if mobility of atoms in clusters is lower together with an enhancement of height of the peak. In contrast, number of atoms with very low mobility or solidlike atoms (and size of their clusters) has a tendency to increase with decreasing temperature and then it suddenly increases in the vicinity of glass transition temperature leading to the formation of a glassy state. A sudden increase in the number of strongly correlated solidlike atoms in the vicinity of a glass transition temperature ( ) may be an origin of a drastical increase in viscosity of the glass-forming systems approaching glass transition. The fact, we find that diffusion coefficient decays exponentially with fraction of solidlike atoms exhibiting a sudden decrease in the vicinity of glass transition region.
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[5] http://dx.doi.org/10.1021/acs.jpcb.5b08912