Potential energy landscape analysis of a continously sheared supercooled model system

Markus Blank-Burian* and Andreas Heuer†

Westfälische Wilhelms-Universität Münster

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Abstract

We performed molecular dynamics simulations of small supercooled binary Lennard-Jones mixtures ($65 <= N <= 1040$) under a constant shear rate. The shearing is achieved by applying Lees-Edwards periodic boundary conditions to the system. The potential energy landscape (PEL) is most informative for small systems. However, we also study the influence of finite size effects on our results.

In previous work, it was shown, that the finite size effects in unsheared systems are limited. The dynamics of these systems can be described by a continous time random walk between minima in the potential energy landscape. Our focus now lies on comparing these results with the constantly sheared system.

The current analysis includes the diffusivity of the particles, the shear viscosity, the energy distribution of the minima and the time between jumps in the minimized potential energy.

*blankburian@uni-muenster.de

†andheuer@uni-muenster.de