Abstract Submitted
for the DFD10 Meeting of
The American Physical Society

Molecular dynamics simulation of non-Newtonian phenomena and shear-induced structural changes in atomic fluids XIN YONG, LUCY ZHANG, Rensselaer Polytechnic Institute — The rheology and microstructure of dense simple fluids have been mysterious subjects for decades due to the lack of direct experimental investigation. In this study, we present a planar Couette flow using molecular dynamics simulations to investigate the properties such as the velocity profile, density distribution, temperature profile and fluid structure within a wide range of wall velocities or shear rates. Here, we examine both boundary-driven shear (with walls) and homogeneous shear (without walls). In the boundary-driven shear, we model a fluid slab confined between two smooth and rigid solid walls. The upper wall is assigned a velocity to induce a planar Couette flow. In the homogeneous shear, only fluid atoms are modeled. The shear flow is generated from a canonical ensemble with a superimposed linear velocity profile associated with the Lees-Edwards periodic boundary conditions. Solid-like fluid layers were observed in the boundary-driven shear. In the homogeneous shear, the string phase is formed at high shear rates, which results in dramatic shear thinning. At lower shear rates, crystallization of fluid atoms induced by a large-scale secondary flow may appear. The physical features of the fluid structures and the corresponding viscosities are compared in the two models.

Xin Yong
Rensselaer Polytechnic Institute

Date submitted: 06 Aug 2010 Electronic form version 1.4