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Structural and Dynamical Heterogeneities in Thin FIlms of a Generic Glass-forming Liquid AMIR HAJI-AKBARI, PABLO G. DEBENEDETTI, Dept. of Chemical & Biological Engineering, Princeton University — Recent discovery of stable glasses by Ediger and coworkers [1] has spurred an interest in structural and dynamical properties of atomic and molecular thin films. Here, we use molecular dynamics simulation to study thin films of a model glass-forming liquid, the Kob-Andersen binary Lennard Jones system [2], and compute profiles of structural properties such as densities, potential energies, stresses and lateral radial distribution functions, as well as dynamical properties such as relaxation times across the film. We observe the liquid to be stratified in the vicinity of the wall, but this stratification is not always accompanied by long-range order. We also observe two distinct dynamical regimes close to the liquid/solid interface. For weakly-interacting walls, a highly mobile region emerges with relaxation times smaller than the bulk, while for strongly-interacting walls, relaxation times can be several orders of magnitude larger in the same region than in the bulk. We are able to establish correlations between density modulations and normal stress modulations, and between relaxation time modulations and lateral stress modulations in the disordered regions of the film.

[1] Swallen SF, et al., Science 315: 353 (2007).
[2] Kob W, Andersen HC, Phys. Rev. E 51: 4626 (1995).

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