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Controlling molecular orientational anisotropy in simulated vapor-deposited glasses[1] IVAN LYUBIMOV, LUCAS ANTONY, JUAN DE PABLO, University of Chicago — It has been shown that stable glasses can be formed via physical vapor deposition on a substrate with the properly tuned temperature. The kinetic stability of vapor deposited glasses has been well investigated, whereas some properties such as the anisotropy of molecular orientation is still not well characterized. We have performed molecular dynamics simulations mimicking the experimental vapor deposition process. The generic coarse-grained model for a small organic molecule reproduces the experimentally observed dependence of molecular orientation on the substrate temperature. The molecular orientation in the glasses changes with the substrate temperature from isotropic at the glass transition temperature, T_g, to slightly normal to the substrate at temperatures just below T_g. For very low substrate temperatures the molecular orientation becomes predominantly parallel to the substrate, as expected. We investigate the mechanism of this behavior and explain the tendency to orient perpendicularly to the substrate in terms of equilibrium liquid properties at a free interface. Our results provide insight into the emergence and role of anisotropic packing in the stability of vapor deposited glasses.

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