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Molecular Dynamics Simulations of Nanomolding Process JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, University of Connecticut — The process of nanomolding hydrophobic monomers and polymers is studied by molecular dynamics simulations. A thin film with a monomer density of 0.524 σ^{-3} consisting of monomers or polymer chains with different degrees of polymerization is prepared by NVT-ensemble simulations. The mold is created by pressing the substrate with attached spherical nanoparticles, representing a master, into thin film. To fix the mold structure the film is crosslinked at different crosslinking densities. The nanoparticle pattern is recovered by molding a similar thin film into the crosslinked mold. The quality of the molding process is evaluated by calculating the eigenvalues of the radius of gyration tensor of the molded nanoparticles as a function of the crosslinking density, degree of polymerization and Lennard-Jones interaction parameters.

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