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Molecular Dynamics Simulations of Nanoimprinting Process JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, Institute of Materials Science, University of Connecticut — Using coarse-grained molecular dynamics simulations we have studied Nanoimprinting Process. The simulations were performed as follows: 1) the master image was created by pressing a substrate with an attached hemisphere, representing the master, into a thin polymeric film. 2) In order to preserve the shape of the master image in the polymeric film, the polymers were cross-linked at different cross-linking densities. 3) The original hemispherical master was replicated by pressing the mold into monomeric liquid. The quality of the molding process was evaluated by comparing the shapes of the original hemisphere and the molded one. We have established how the differences between the original and replica depend on the size of the master, the fraction of the cross-links, the network shear modulus and the master mold-monomer liquid affinity, which is controlled by the parameters of the Lennard-Jones potential.

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