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Molecular dynamics simulation study of the ejection and transport of polymer molecules in matrix-assisted pulsed laser evaporation LEONID ZHIGILEI, ELODIE LEVEUGLE, University of Virginia — There are a number of applications that utilize the ability of laser ablation of a volatile matrix to entrain, eject and, if needed, deposit large macromolecules to a substrate with minimum chemical modification. In particular, the Matrix-Assisted Pulsed Laser Evaporation (MAPLE) technique is used in fabrication of ultra-thin organic films for optoelectronic, biomedical, and chemical sensor applications. In this presentation we report the results of a computational investigation of the mechanisms of molecular ejection in MAPLE. Coarse-grained molecular dynamics simulations are performed for polymer concentrations up to 6 wt.%. Contrary to the original picture of the ejection and transport of individual polymer molecules in MAPLE, the simulations indicate that polymer molecules are only ejected as parts of polymer-matrix clusters/droplets generated in the process of the explosive disintegration of the overheated matrix. An internal release of matrix vapor in the overheated droplets is shown to be capable of pushing polymer molecules to the outskirts of the droplets, forming "molecular balloons" in which polymer-rich surface layers enclose the volatile matrix material. The results of the simulations explain some of the complex morphologies observed in polymer films deposited in MAPLE and conventional polymer ablation/deposition experiments.

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