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Dewetting of nanometer-sized thin films on a solid substrate: A large-scale simulation study TRUNG NGUYEN, MIGUEL FUENTES-CABRERA, JASON FOWLKES, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, JAVIER DIEZ, ALEJANDRO GONZALEZ, Universidad Nacional del Centro de la Provincia de Buenos Aires, Tandil, Argentina, LOU KONDIC, New Jersey Institute of Technology, Newark, New Jersey, United States, W. MICHAEL BROWN, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, PHILIP RACK, University of Tennessee, Knoxville — Directing the assembly of nanoparticles into ordered arrays using interfacial instability has been of practical interest. Recent experimental and theoretical studies have revealed the role of the Raleigh-Plateau instability in determining the breakup process of fluidic thin films deposited on a solid substrate. Using all-atom models, we investigate the dynamic behavior of nanometer-sized thin rings as a function of initial geometry in the presence of Raleigh-Plateau-type instability and inward pressure due to initial azimuthal curvature. We consider systems at close-to-experiment scales consisting of hundreds of thousands to millions of atoms using LAMMPS, a massively parallel molecular dynamics package, with GPU acceleration. The simulation results are shown to be consistent with continuum modeling calculations in predicting the fastest growth mode and breakup times, both of which are important to the evolution of the thin films. Our study serves to stimulate future investigations connecting experimental and theoretical findings towards fabricating ordered arrays of nanoparticles.

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