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Breakup of Liquid Nano-threads Simulated by Molecular Dynamics HARRIS WONG, PING DU, Department of Mechanical Engineering, Louisiana State University, Baton Rouge, Louisiana, USA — A circular liquid thread of radius R will break up into drops if the axial wavelength of surface perturbation $L > 2\pi R$. If $L < 2\pi R$, the thread is stable and will remain intact. This is Rayleigh's stability criterion based on a continuum model. We use molecular dynamics to simulate the evolution of Lennard-Jones liquid threads with equilibrium radius R = 2.25-6.59, where R has been non-dimensionalized by the distance at which the Lennard-Jones potential equals zero. Periodic conditions are imposed at the boundaries of the simulation box so that the thread length is the wavelength L. We find that if R is fixed, there exists a range of L bounded by L_{min} and L_{max} such that for $L \geq L_{max}$ the thread always breaks up into drops and stays as drops, and for $L \leq L_{min}$, the thread remains connected but the shape varies continuously among a series of shapes including a cylinder, unduloids, and sinusoids. For $L_{min} < L < L_{max}$, the thread can break up temporarily into drops and then resume connected. As R increases, $L_{min} \rightarrow L_{max}$, and L_{max} is slightly smaller than $2\pi R$. The appearance of various shapes can be explained by the energy fluctuation of the system.

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