Abstract Submitted
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Simulating instabilities of liquid metal alloys on nanoscale using molecular dynamics simulations.[1] RYAN ALLAIRE, New Jersey Institute of Technology, MIGUEL FUENTES-CABRERA, Oak Ridge National Laboratory, PHILIP D. RACK, The University of Tennessee, Knoxville, LINDA CUMMINGS, LOU KONDIC, New Jersey Institute of Technology — Classical molecular dynamics simulations are used to investigate the influence of phase separation of liquid metal alloys on Rayleigh-Plateau (RP) type instabilities of free standing alloys, as well as alloys deposited as films on substrates. The alloy geometries are created in thin strips with widths modulated by sinusoidal waves of varying amplitudes and wavelengths, corresponding to the fastest growing mode obtained from continuum RP theory. We explore the influence of temperature on the breakup process and on phase separation. Both the ratio of phase separation length scales to wavelengths of the sinusoidal perturbations, and the initial location of phase separation are found to influence the RP instability development, either by modifying the instability growth rate or by changing the spatial positioning of the breakup point. As an outcome, nanoparticles are formed, characterized by morphologies of either core-shell or layered type. Growth rates of instabilities are compared to the predictions of RP theory and resultant nanoparticle compositions are analyzed.

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