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KINETICS MODEL OF BREAKUP OF NANOWIRES AND NANOCONES INTO CHAINS OF NANOPARTICLES

A kinetic Monte Carlo approach is applied to studying shape instability of nanowires and nanocones that results in their breaking up into chains of nanoparticles. Our approach can be used to explore dynamical features of the process that correspond to experimental findings, but that cannot be interpreted solely by continuum modeling reminiscent of the description of the Plateau-Rayleigh instability in liquid jets. For example, we observe long-lived dumbbell-type fragments and other typical non-liquid-jet characteristics of the process, as well as confirm the observed lattice orientation dependence of the breakup process of single-crystal nanowires. We provide snapshots of the process dynamics, and elaborate on the nanowire-end effects, as well as on the morphology of the resulting nanoparticles.

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