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3D Lattice Boltzmann Modeling of Nanoparticle Self-Assembly in Evaporating Droplets and Rivulets MINGFEI ZHAO, XIN YONG, Binghamton University — In this work, a three-dimensional free-energy-based multiphase lattice Boltzmann method-Lagrangian particle tracking hybrid model is presented to simulate nanoparticle-laden droplets and rivulets undergoing evaporation. The 3D model enables the development of the 3D flow structures in the evaporating droplets, as well as allows us to capture the axial flows in the evaporating rivulets. We first model non-evaporating droplets and rivulets loaded with nanoparticles and the effects of particle-fluid interaction parameters on particle dynamics are characterized. By implementing evaporation, we probe the self-assembly of nanoparticles inside the fluid mass or at the liquid-vapor interface. The 3D microstructure of nanoparticle assemblies is quantified through radial distribution functions and structure factors. In particular, the final deposit of evaporating rivulets with oscillatory axial flows is revealed, resembling the flow field in printed rivulets in experiments. Our findings offer a theoretical framework to explore the dynamics of nanoparticle self-assembly in evaporating fluid mass.

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