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Molecular dynamics simulations of the evaporation of particle-laden drops WEIKANG CHEN, JOEL KOPLIK, ILONA KRETZSCHMAR, City College of CUNY — We use molecular dynamics simulations to study the evaporation of particle-laden droplets on a heated surface. The droplets are composed of a Lennard-Jones fluid containing rigid particles which are spherical sections of an atomic lattice, and heating is controlled through the temperature of an atomistic substrate. We observe that sufficiently large (but still nano-sized) particle-laden drops exhibit contact line pinning, measure the outward fluid flow field which advects particle to the drop rim, and find that the structure of the resulting aggregate varies with inter-particle interactions. In addition, the profile of the evaporative fluid flux is measured with and without particles present, and is also found to be in qualitative agreement with earlier theory. The compatibility of simple nanoscale calculations and micron-scale experiments indicates that molecular simulation may be used to predict aggregate structure in vaporative growth processes.

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