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Two-step nucleation: Monte Carlo simulation of heterogeneous nucleation of liquid droplets on soluble nanoscopic aerosols OLEKSANDR ZAVALOV, SOPHIE MCGIBBON-GARDNER, PETER POOLE, Department of Physics, St. Francis Xavier University, Antigonish, Nova Scotia, Canada, RICHARD BOWLES, Department of Chemistry, University of Saskatchewan, Saskatoon, Saskatchewan, Canada, IVAN SAIKA-VOIVOD, Department of Physics and Physical Oceanography, Memorial University of Newfoundland, St. John's, Newfoundland, Canada — We use a 2D Ising lattice gas model to conduct Monte Carlo simulations of the heterogeneous nucleation of a liquid droplet from the supersaturated vapor phase, as triggered by a soluble nanoscopic aerosol particle. The liquid droplet that forms is a cluster of both solvent and solute particles. As a function of the size n of the droplet, we observe a solubility transition: At smaller n, the droplet consists of a compact solute cluster wetted by solvent, while at larger n the solute dissolves and is more uniformly distributed within the droplet. We evaluate the free energy of formation of a droplet as a function of n, and identify conditions at which nucleation is a two-step process. That is, two free energy barriers are encountered as the droplet grows, one associated with the solubility transition, and the other with the nucleation of the bulk solvent phase. We also evaluate the nucleation rate from the mean first passage time for the droplet to reach the critical size for the formation of the bulk phase, and quantify the influence on the rate due to solute solubility, and due to the relative heights of the barriers for the solubility and bulk transitions.

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