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Structure in Binary Nanodroplets HONG XIA NING, GERALD WILEMSKI, University of Missouri-Rolla — Recent SANS measurements of core-shell structure in binary nanodroplets ($\sim$ 9 nm) have stimulated our research on the structure of droplets of this size. [Wyslouzil, et. al., Phys. Chem. Chem. Phys. **8**, xxx, (2006)] By structure, we mean the spatial distribution of chemical species within the droplet. Based on recent work by Cordeiro and Pakula [J. Phys. Chem. **109**, 4152 (2005)], we developed an efficient Lattice Monte Carlo (LMC) method to simulate binary droplets containing 5000 to 10000 particles. Simulations of nanodroplets of various compositions were made to study phenomena such as species segregation and phase separation. Depending on the relative strengths of the intermolecular interactions, various interesting structures were found. Droplets may be fairly well-mixed, strongly segregated core-shell structures, or even highly segregated nonspherical shapes resembling partially disassembled Russian dolls. We explored the temperature dependence of the droplet structures and observed that the reversible change between the core-shell and Russian doll structures could be viewed as a wetting—dewetting transition. The transition temperature was determined for a specific system.

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