OUT-OF-EQUILIBRIUM SELF-ASSEMBLY OF BINARY MIXTURES OF NANOPARTICLES

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A coarse-grained lattice-gas model is developed to study drying-mediated self-assembly of binary mixtures of nanoparticles. Out-of-equilibrium simulations of the model provide insight into the dynamics of solvent evaporation and the formation of self-assembled superstructure domains. Three model systems are considered, corresponding to equilibrium phase separation between nanoparticles of type A and B, to an amorphous state, and to an ordered, checkerboard-like, superstructure. Interestingly, the mechanism for self-ordering depends on the nature of equilibrium superstructure and on the dynamical coupling to the evaporating solvent. In a certain limit of evaporation, the system shows complex behavior common to arrested micro-phase separation of glassy materials. Several qualitative features are discussed and scaling laws for the growth of domains are determined numerically.