Abstract

Binary nanoparticle superlattices or BNSL's have been a major area of research in nanotechnology for the last decade. The conventional lithographic techniques are limited to fabricate features only within a plane while these self-assembled structures are formed within a given volume. The potential applications of self-assembly leading to crystalline structures include nanoelectronics, photonics and improving the fundamental understanding of the bottom-up approach as well. The present work deals with the crystallization of nanoparticles in a colloidal suspension leading to three dimensional crystals(BNSL's).

The goal is to generate phase diagrams for binary nanoparticle suspensions with varying charge ratios between the two particles. Monte Carlo molecular simulations in various equilibrium ensembles are the basis for the generation of equations of state and calculation of free energies of the two coexisting phases. Coexistence here implies the solid-fluid thermodynamic equilibrium and consequently the equivalence of free energies. The calculation framework is standard for pure substances, but advanced techniques need to be used for mixtures. The focal point of this work is the effect of charge asymmetry on the formation and stability of BNSL's from the binary suspension.

There are six phase diagrams for charge ratios of 0, 0:2, 0:4, 0:6, 0:8 and 1:0. The variables are the reduced pressure P_ and the mole fraction XA. The proposed applications of BNSL's are generally dependent on substitutional order. From the results, symmetric mixtures are favorable for the formation of BNSL's while charge asymmetry gives rise to solid solutions.