

Abstract Submitted
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Phase Equilibrium of Size-Dispersed Colloid Systems with soft pair interactions: A Monte Carlo Study IOANNIS BITSANIS, FORTH-IESL, Heraklion, Greece, IOANNIS ECONOMOY, MARIANNA YIANNOURAKOU, NR-CPS “Demokritos”, Ag. Paraskevi, Greece — We have studied the solid-fluid coexistence for systems of polydisperse soft spheres that interact via power-law potentials. We employed isobaric semi-grand ensemble simulations. Gibbs-Duhem integration traced the coexistence pressure as a function of the variance of the imposed activity distribution. Fluid-solid coexistence densities were determined to be monotonically increasing functions of the breadth of particle size dispersity. Our simulations testified to the existence of terminal diameter dispersity, i.e a dispersity above which there can be no amorphous-crystalline phase coexistence. At the terminus, size-dispersity increases from 5.8% to 6.7% for the crystalline phase as pair interactions soften. The crystalline phases’ allowable size dispersity is enhanced by potential softness, while the dispersity of the amorphous (liquid) phases follows an opposite trend. Overall, the 2 phase region shrinks monotonically and substantially as colloid-colloid interactions soften. Furthermore, amorphous phases accommodate, on average, smaller particles than those of the ordered (fcc) phase. Crystalline phases composed of size disperse particulates exhibit a higher degree of local order than their mono-disperse counterparts, admittedly at differing thermodynamic conditions. GSRT-ENTER

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