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Brownian dynamics simulations of insulin microspheres formation WEI LI, Lehigh University, AMIT CHAKRABARTI, Kansas State University, JAMES GUNTON, Lehigh University — Recent experiments have indicated a novel, aqueous process of microsphere insulin fabrication based on controlled phase separation of protein from water-soluble polymers. We investigate the insulin microsphere crystal formation from insulin-PEG-water systems via 3D Brownian Dynamics simulations. We use the two component Asakura-Oosawa model to simulate the kinetics of this colloid polymer mixture. We first perform a deep quench below the liquid-crystal boundary that leads to fractal formation. We next heat the system to obtain a break-up of the fractal clusters and subsequently cool the system to obtain a spherical aggregation of droplets with a relatively narrow size distribution. We analyze the structure factor S(q) to identify the cluster dimension. S(q) crosses over from a power law q dependence of 1.8 (in agreement with DLCA) to 4 as q increases, which shows the evolution from fractal to spherical clusters. By studying the bond-order parameters, we find the phase transition from liquid-like droplets to crystals which exhibit local HCP and FCC order. This work is supported by grants from the NSF and Mathers Foundation.

Wei Li
Lehigh University

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