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Crystal Growth in Lennard-Jones Mixtures: A Model System to Study Generic Effects in Biomineralization Processes MARC RADU, KURT KREMER, Max Planck Institute for Polymer Research — In various scientific fields regulating the growth of crystalline structures and tuning their morphologies plays an important role. E.g. in pharmaceutical delivery the crystallization of a supersaturated drug solution is inhibited by the addition of stimuli-responsive polymers. While past simulation studies rather focused on a detailed understanding of the binding modes of specific additives to likewise specific crystal surfaces here we investigate the characteristics of a generic model system in which we modify the growth mechanisms and the emerging shapes of Lennard-Jones crystallites by tuning the specific interaction parameters and/or adding polymer chains - represented by linear bead-spring molecules - to the system. We performed molecular dynamics simulations on samples containing a crystalline phase embedded in a supersaturated solution applying an adaptive simulation scheme in order to keep the chemical potential difference between the solid and the surrounding liquid constant. We report on different crystal properties depending on a systematic variation of simulation parameters as the solvent content, the solubility and the density of polymer chains. We analyze our results by means of various approaches within the framework of non-equilibrium statistical physics.

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