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Phase behavior and crystal nucleation and growth in a system of short semi-flexible chains[1] BART VORSELAARS, DAVID QUIGLEY, Univ of Warwick — A system of semi-flexible short chains is simulated to study its phase behavior and ability to crystallize, by using a combination of molecular dynamics and other techniques. For calculating the free energy of the liquid phase a new method is introduced. It is very simple to implement in practice and leads to accurate computation of the melting curve. Furthermore we determine the rate of nucleation and crystal growth in this system via a combination of path-sampling and brute-force simulation techniques. By comparing these quantities, we infer the initial microstructure of the solid phase. Due to the strong anisotropy in the crystal growth rate grains no thicker than a single chain are common, even at moderate supercoolings.

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