

Conformational transitions of flexible polymers

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We investigate collapse and crystallization of flexible homopolymers by means of multicanonical computer simulations of a simple off-lattice bead-spring polymer model with FENE (finitely extensible nonlinear elastic) bond potential [1] and intramonomeric Lennard–Jones interaction. Beside the well known Theta transition we also observe another cross-over at lower temperatures which is expected to be the liquid-solid transition. This is indicated by sharp energetic fluctuations as signaled by the specific heat. The crystallized polymer structures possess similarities to ground states of pure Lennard-Jones clusters. From our results, we also conclude that crystallization and collapse transition remain well separated in the thermodynamic limit [2].

[1] R. B. Bird, C. F. Curtiss, R. C. Armstrong and O. Hassager, *Dynamics of Polymeric Liquids*, 2nd ed., 2 vols. (Wiley, New York, 1987).

[2] D. F. Parsons and D. R. M. Williams, *J. Chem. Phys.* 124, 221103 (2006); *Phys. Rev. E* 74, 041804 (2006).