

MIT Chemical Engineering Department Special Seminar

Molecular dynamics simulation of polymer crystallization: network formation in polyethylene fibers and chiral (polymorph) selection in helical polymers



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Crystallization is a process dominating structures, morphologies, and physical properties of every crystalline polymer. Besides its great significance in technology and relevance to biology, it is very fascinating by itself to understand the emergence of crystalline order from the entangled web of macromolecules. Despite intensive investigations for more than half a century, experimental knowledge about the molecular pathways to the crystalline state are still far from satisfactory. With the recent progress in computer modeling, however, we have a very promising tool in hand to directly observe crystallizing polymers. I will here introduce some topics, of our recent interest, about the computer modeling of polymer crystallization. We here consider both simple linear polymers such as polyethylene and model helical polymers such as polypropylene¹⁾.

Rapid crystallization of polymers during uniaxial stretching or shear deformation is known to allow "in situ" observation of the molecular processes of fiber formation. Adopting this well-acknowledged approach, we are reexamining²⁾ various aspects of fiber crystallization in polyethylene, such as nucleation and growth, formation of networks made of crystallites and connecting chains (tie molecules), and also possible relevance of intermediate crystalline phases. On the other hand, in helical polymers, crystallization always goes with clear polymorph selection of usually definite crystal chirality. However, their molecular mechanisms almost lie hidden, despite great scientific interest. I also want to talk about our recent efforts, though preliminary, to directly observe chiral crystallization in helical polymers, expecting to share interest about this nearly forgotten subject of polymer simulation³⁾.

References

- 1) T. Yamamoto, et al. *Molecular dynamics modeling of polymer crystallization; from simple polymers to helical ones*, Faraday Discussion **128**, 75 (2005)
- 2) T. Yamamoto, *Molecular dynamics in fiber formation of polyethylene and large deformation of the fiber*, Polymer **54**, 3086 (2013)
- 3) T. Yamamoto, *Molecular Dynamics of Crystallization in a Helical Polymer Isotactic Polypropylene from the Oriented Amorphous State*, Macromolecules **47**, 3192 (2014)