ΕΛΕΠ

Hellenic Polymer Society

ELEP SEMINAR

Friday 30/06/2023 at 17:00 (Greek Time)

https://us02web.zoom.us/j/83209658623?pwd=clZtWTFGc3dzR1RmdkdMSkxEQ2dCUT09

Meeting ID: 832 0965 8623 Passcode: 356967

Playing with entanglements to structure polymer materials

Prof. Kurt Kremer

Director, Theory Department

Max Planck Institute for Polymer Research

kremer@mpip-mainz.mpg.de

Abstract

Entanglements are known to dominate the rheological properties of long chain polymer melts and dense solutions. Their properties and consequences lead to the generally well established reptation/tube model, which is at the basis of our understanding of many properties and processes. However, beyond analyzing their effects and understanding the very nature of entanglements, one also takes the approach to use them to manipulate and structure materials. The lecture will give a few such examples ranging from melts of non-entangled long polymer chains[1] and the questions of the glass transition temperature T_g, ring melts[2] and the role of topological constraints in passive and active systems to expanded free standing films[3]. While the first two topics predominantly contribute to our basic understanding, thin polymer films have attracted much attention due to their usefulness as supporting media in tissue engineering or as membranes in separation processes. Thus, a simulation guided processing is highly desirable. However, equilibrating free-standing films of highly entangled polymer melts is a challenge for computer simulations. We approach this problem by a hierarchical approach, where polymer melts based on a very coarse-grained soft-sphere model (first) confined between two repulsive walls are systematically fine grained. This is done until the underlying microscopic details of the employed bead-spring model are reached. We use a version of the model, which allows for free surfaces and a systematic investigation of the glass transition[4,5]. A detailed study of the glass transition temperature as a function of film thickness is underway. Starting from this, biaxially expanded films and the role of entanglements on their morphology are investigated. Motivated by the simulations, a similar process is applied experimentally on films of highly entangled polystyrene. Our results show excellent qualitative and even semi-quantitative agreement.

---

[1] M. K. Singh et al., *Macromolecules* **53**, 7312 (2020).

[2] J. Smrek et al., *Nat. Comm.* **11**, 26 (2020).

[3] H.-P. Hsu et al., *Adv. Sc.* (2023). DOI: 10.1002/advs.202207472

[4] H.-P. Hsu and K. Kremer, *J. Chem. Phys.* **150**, 091101 (2019).

[5] H.-P. Hsu and K. Kremer, *J. Chem. Phys.* **153**, 144902 (2020).

Kurt Kremer

Director, Theory Department
Max Planck Institute for Polymer Research
55128 Mainz, Germany
E-mail: kremer@mpip-mainz.mpg.de
Webpage: https://www.mpip-mainz.mpg.de/de/kremer

Short Bio

Professor Kurt Kremer joined the Max-Planck Society in September of 1995 as the sixth director of the Max-Planck Institute for Polymer Research, heading the newly established theory group. After studying physics, he received his PhD in 1983 from the University of Cologne under the supervision of Prof. Binder, working at the National Research Center KFA Jülich. He performed computer simulations for dynamic and static properties of polymers in bulk and near surfaces. After spending another year at Jülich he moved for a post-doctoral stay to Exxon Research and Engineering Corporation, USA, working on polymers and on charge stabilized colloids in collaboration with Drs. Grest, Pincus, and others. Being back in Germany he obtained his Habilitation in 1988 at the University of Mainz. After that, he returned to the solid state laboratory of the KFA Jülich as senior scientific staff. He spent several extended visits as visiting professor/scientist at Exxon Research (Dr. Grest), UC Santa Barbara (Materials Dept., Prof. Pincus), and University of Minnesota (Dept. Chem. Engineering and Materials Science, Profs. Davis, Bates, Tirell, and others). After a short stay at the central research department of the Bayer AG, Leverkusen, he moved to the Max Planck Institute for Polymer Research.

Professor Kremer's research concentrates on statistical and computational physics and physical chemistry of soft matter. Specific current research areas of the theory group include computational physics methods/ applications, statistical mechanics of soft matter (polymers, colloids, membranes...), structure process property relations as well as multiscale modeling of synthetic and biological soft matter.

Awards

- 2022: Berni J. Alder CECAM Prize
- 2022: SPSJ International Award
- 2018: Elected member of the Academia Europaea
- 2016: J. D. Ferry Lecture, University of Wisconsin
- 2016: Elected member of the European Academy of Sciences, EurASc (Brussels, Belgium)
- 2012: Elected member of the German National Academy of Sciences Leopoldina (Deutsche Akademie der Naturforscher Leopoldina, Halle, Germany)
- 2012: KITP (UC Santa Barbara) Distinguished Scholar
- 2011: Polymer Physics Prize, American Physical Society
- 2011: Honorary Professor of Physics, University of Heidelberg
- 2006: Fellow, American Physical Society
- 2006: Nakamura Lecturer, UC Santa Barbara
- 1999: Whitby Lecturer, Akron University
- 1992: Walter Schottky Prize of the German Physical Society
- 1991: George T. Piercy Distinguished Professor of Materials Science and Chemical Engineering, University of Minnesota