September 15,
16:00-17:00
E-R2-2027

Computational
Materials
Science

Seminar

UHMWPE polymerization and fiber formation: computer simulations

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Speaker introduction

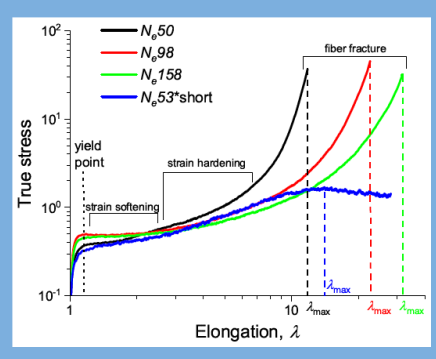
Alexander Chertovich recieved degree in physics from Lomonosov Moscow State University in 2001, on the Chair of Polymer and Crystal Physics, supervised by Prof. A.khokhlov. In 2003 he defended his Ph.D. thesis on the topic “Computer simulation of Biomimetic copolymers” at the same place. Was a visiting reseacher in DTU (Denmark) and UniUlm (Germany). In 2019 he moved to Semenov federal Research Center for Chemical Physics. His scientific interests cover the fields of physics and chemistry of polymers, composites, as well as electrochemical devices.

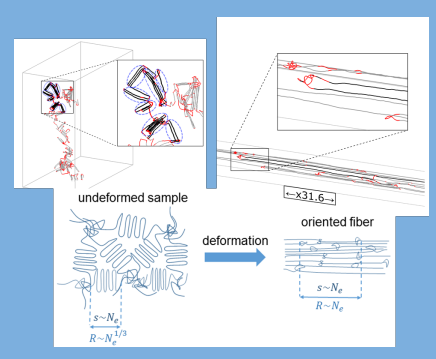
Seminar abstract

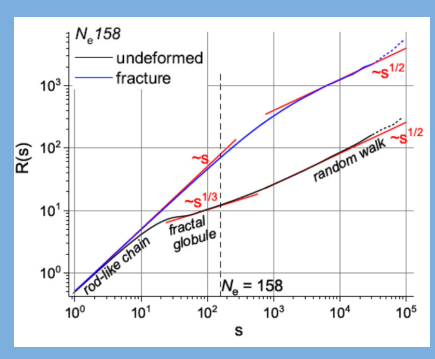
Polymer fibers consist of macromolecules oriented along the fiber axis. Better alignment of chains leads to an increased strength of the fiber. It is believed that the key factor preventing formation of a perfectly oriented fiber is the chain entanglements. We performed large-scale computer simulations of polymerization and uniaxial stretching of semicrystalline ultrahigh molecular weight polyethylene (UHMWPE). As a synthesis model, we consider homogeneous catalysis; for fibers processing we consider drawing from the melt. We assessed how the rate of polymerization and the concentration of initiators affect entanglement of chains. We discovered that there is an optimal number of entanglements per macromolecule necessary to maximize chain orientation in a fiber. Polymers that are entangled too strongly form less-oriented fibers. On the other hand, when polymers have too few entanglements per chain, they disentangle during stretching, and a strong fiber is not formed.

References:

[1] A. Petrov, P.Kos, V. Rudyak, A. Chertovich, Macromolecules 2020, 53, 16, 6796.
[2] A. Petrov, V. Rudyak, A. Chertovich, Macromolecules 2022, 55, 15, 6493.







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