INSTITUTE OF MACROMOLECULAR CHEMISTRY AS CR

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

10 - 14 JULY 2016 PRAGUE

SELF-ASSEMBLY IN THE WORLD OF POLYMERS

80th PRAGUE MEETING ON MACROMOLECULES

BOOK OF ABSTRACTS AND PROGRAMME

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COARSE-GRAINED COMPUTER SIMULATION OF CRYSTALLIZATION IN POLYIMIDE MELTS

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Crystallization in polyimides melts plays a key role in their characteristics. The degree of crystallinity, depending on type of particular polyimide material, could either improve the mechanical properties (modulus increase) or lead to larger deterioration (increasing of brittleness). In this work we study behavior of two polyimides which are based on 1,3-bis-(3',4-dicarboxyphenoxy)-benzene (dianhydride R) and various types of diamines:4,4'-bis-(4''-aminophenoxy)-diphenylsulfone (diamine BAPS) and 4,4'-bis-(4''-aminophenoxy)-diphenyl (diamine BAPB) [1]. The main structural difference of these polyimides is the presence of an additional SO_2 group in the R–BAPS diamine fragment compared to the R–BAPB one. This modification of the polymer chain leads to decrease of the persistence length, and as a result to increase of the flexibility of R-BAPS diamine fragment. We have developed and parameterized coarse-grained models for each of two types of the polyimides, semi-crystalline and amorphous one. All calculations have been carried out by means of dissipative particle dynamics simulations [2].

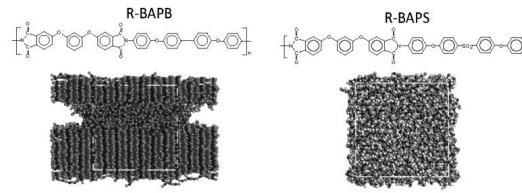

Fig. 1. Chemical structures of the repeating units (at the top) and morphologies (at the bottom) of thermoplastic heat-resistant polyimides R–BAPB (on the left) and R–BAPS (on the right).

[1] S. V. Larin, S.G. Falkovich, V. M. Nazarychev,A. A. Gurtovenko, A. V. Lyulin,S. V. Lyulin, RSC Adv. 4: 830, 2014.
[2] R.D. Groot, P.B. Warren, J. Chem. Phys. 107: 4423, 1997.