

Preface

The 3rd International Symposium "Molecular Mobility and Order in Polymer Systems" continues the series of Saint-Petersburg meetings organized by the Institute of Macromolecular Compounds of Russian Academy of Sciences (RAS) and the Department of General and Technical Chemistry of RAS. The Symposium was sponsored by the International Union of Pure and Applied Chemistry and supported by the Russian Foundation of Basic Research and St. Petersburg Research Center of RAS.

The present Symposium (as well as the first one in 1994) was oriented more towards dynamical and relaxation phenomena whereas the discussion at the previous 2nd Symposium (May, 1996) was mainly focused on the problems of structure and order. Of course, these shifts in the subject of Symposiums were never too dramatic: mobility in polymer physics and physical chemistry, just like in real life, is inseparable from the order (or disorder!) of the system.

The main topics of the Symposium include:

- conformation and mobility of macromolecules in solutions, melts, and networks in strong external fields
- structure and properties of liquid-crystalline polymers
- block copolymers
- polymer layers, brushes and micelles
- polymer complexes and membranes
- structure and dynamics of branched polymer systems, stars, dendrimers and networks

All the systems considered share a common general feature: the order present in them is "soft", and there exists a pronounced molecular mobility.

The Symposium included 18 invited plenary lectures, 32 contributed lectures and 180 poster presentations. This meeting was a truly international one: lectures and posters were submitted by scientists from Canada, Czech Republic, Finland, France, Germany, Greece, Hungary, Italy, Israel, Japan, Kazakhstan, Lithuania, The Netherlands, Portugal, Russia, Spain, Sweden, Turkey, USA, Uzbekistan, Ukraine, and UK.

A short account of the materials presented at the Symposium was published in the Book of Abstracts.

The plenary and contributed lectures were presented by eminent scientists, classics of polymer science (Sam Edwards, Tatiana Birshtein, Victor Kabanov ...), and also by well-known active researchers of younger generations.

The Symposium featured a dynamic poster session which included presentations by many participants, especially young scientists, and was accompanied by very lively discussions.

Regrettably, this volume does not cover all the new and interesting results discussed at the Symposium since not all the authors were able to present their lectures for publication in this volume (some of the materials had been published earlier or submitted elsewhere). However, it provides a good representation of the scope of the meeting and the main topics of the discussion.

Because of the close interconnection between the different topics we preferred a less detailed classification of papers than that given in the original topics of the Symposium. The classification accepted in this Volume i.e. "Mobility-Structure-Order" or "Structure-Order-Properties" is still of a somewhat conditional character and is based on the most characteristic features of the investigation in a given paper.

Mobility-Structure-Order

The lectures devoted to polymer dynamics describe various types of relaxation phenomena on different time and length scales (from nano-scale to macroscopic) investigated by a broad variety of experimental, theoretical and computer simulation methods. Polarized luminescence provides information on the molecular mobility in the nanosecond range which can be used to characterize molecular structure for copolymers of various chemical structure (Anufrieva et al.). An extensive set of methods: DSC, interferometric spectroscopy, TGA, dielectric relaxation spectroscopy, and thermally stimulated depolarization were applied to study molecular dynamics in nano-structured polyimidesilicon materials (Bershtein et al.). Dybal and coworkers investigated the structure and mobility in polycarbonates and polycarbonate-PEO mixtures by NMR and vibrational spectroscopy. The relaxation of poly(4-oligodimethylsiloxanyl) styrene as seen by solid state ^{29}Si NMR was discussed by Kawakami in connection with the gas permeation behavior of the polymer membranes. Quasi-elastic neutron scattering, X-ray and dielectric spectroscopy were applied to the investigation of the super-structure, order and segmental dynamics of carbosilane dendrimers in bulk and solution (Stuehn et al.). Mechanical strength, ion conductivity, gas permeability, and ion exchange capacity were studied for new polymer membranes used for low-temperature fuel cells (Sundholm et al.). Rheo-optical FT-IR spectroscopy was used for investigating the intra- and intermolecular hydrogen-bonding and its effect on the local mobility in solid poly(acrylic acid) films (Mavinkurve and Heyvelmans-Wijdenes). The mechanical and electrical degradation processes of polymer composites and the application of the Zhurkov thermofluctuation theory were studied by Mamedov et al.

Some papers were devoted to the theory and computer simulation of the molecular mobility. The theoretical approach to the viscoelasticity of polymer melt and cross-linked system as a function of frequency and cross-linking was developed by Edwards and Takano in the framework of tube model. The topology of the system and closing of the tube at cross-links were taken into account. The influence of the long-range hydrodynamic interactions between polymer network and effective viscous medium on the cooperative relaxation spectra was considered by Gotlib. Borodin and Khazanovich proposed a non-standard alternative approach to hydrodynamic interactions in polymer solutions applied to the calculation of the diffusion coefficient and intrinsic viscosity of polymer solutions. An application of the mode-coupling theory to the dynamics of the DNA macromolecules and proteins and its effects on the NMR relaxation was treated by La-Penna and coworkers. Fatkullin and Kimmich considered the problems of intra- and interchain relaxation in entangled polymer melts using memory function formalism and

treated also the visco-elastic properties of polymer melts with the help of renormalized Rouse formalism. Ngai presented an improved theory of the concentration dependence of the cooperative polymer dynamics in solutions based on the general coupling model explaining the stretched exponential time dependence of correlation functions and the same type of the stretched exponential dependence of relaxation times on concentration. The conformational change and the kinetics of the coil-stretch transition in polymer chains in a steady elongational flow were investigated by computer simulation (de la Torre and Cifre). Oleinik and coworkers performed a detailed computer modeling of the local structure and rotational mobility of ethylene- α -olefin copolymers in n-paraffin crystals.

Thus the theoretical work and computer simulations emphasize a detailed study of the collective motions in complex many-chain systems and the effects of strong external or internal fields (as in crystalline phases).

Structure-Order-Properties

The papers of this part of the Symposium were devoted to the study of the interconnection between chemical constitution, morphology and order for a broad class of macromolecular systems mentioned in the topics of the Symposium. New types of mesophases (e.g., aperiodic layer mesophases) in rigid-chain copolymers and co-(poly)esteramides appearing in the two-phase semicrystalline materials were considered by Antipov, Plate, and Levchenko. Experimental electron microscopic structure investigations of organic molecules with non-linear optical properties and ab initio quantum-mechanical structure determination were carried out by Voigt-Martin and coworkers. In the paper of Koyun et al. the effects of the molecular and supermolecular structure of polyolefin on some mechanical properties of plastics used for manufacturing pipes were investigated. The structure of hydrophobically modified poly(ethylene oxide), association and ordering effects, formation of aggregates and rheological behavior was considered by Francois et al. The interconnection between the polymer structure and optical properties (in IR and UV spectra) for polymer composite films was investigated by Boydag et al. Zaitsev and coworkers have studied the structure and properties of polymethylsiloxane monolayers with styrene and polystyrene-polysiloxane latexes and monolayer films. The group of papers was devoted to the properties of the neutral and charged hydrogels, their interaction with incorporated particles and surfactants (Starodoubtsev, Khokhlov et al.), the complexes between gels and organic dyes (Nasimova, Makhaeva, Khokhlov) and problems of the ion aggregation in hydrogels (Philippova, Khokhlov et al.).

Theory and computer simulation of the structure-order problem was also represented extensively on the Symposium. The theory of mixed superstructures with different morphology formed in mixtures of ABC-triblock and AB-, AC- and BC-diblock polymers was presented by Birshtein, Amoskov and Polotskii. Johner, Vilgis and Joanny considered the behavior of polyelectrolyte gels in poor solvent chain on the basis of the single chain elasticity using the necklace model of polyelectrolyte. Paul, Weber and Binder considered the competition between local LC-ordering and glassy-freezing in melts of semiflexible polymers using the MC computer simulation of the bond-fluctuation model. A simulation of a specific structur-

ally ordered phase intermediate between the crystalline and amorphous phases was performed by Ludovice et. al. Conformational structure and some dynamic characteristics of charged polyelectrolyte brushes (anchored chains) were studied by molecular dynamics method by Seidel and Csaika. Lukasheva, Darinskii et al. studied (by molecular mechanics method) the conformation of polyisocyanates with helical structure, investigated the mechanisms of helix reversal and the comparative role of breaks and librations in the chain flexibility of PIC. The microstructure and collapse transition of protein-like AB-copolymer globules was investigated by computer simulation by Ivanov et al.

This brief review of the materials of the Symposium including those presented in this volume shows that the main interest in the investigation of the “structure-order-properties” problem lies in the domain of systems with complex chemical constitution and morphology like polyelectrolytes, copolymers, mesophases, glassy states with local ordering etc.

We believe that the 3rd International Symposium contributed significantly to the understanding of the interconnection of mobility and order in the polymer systems.

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