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Mission and challenges of polymer science and technology*

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Abstract: Following the first IUPAC Polymer Conference on the Mission and Challenges of Polymer Science and Technology (IUPAC PC2002), this article highlights and summarizes the historical development of polymer science and technology and the recent advances that have occurred and are occurring in the subject. It highlights the mission and challenges for the future, particularly as reflected in the papers presented at the conference and in the conference's concluding panel discussion. The important role of IUPAC in defining and leading developments in polymer science and technology is also described. The central role of polymer science and technology and its close interactions with chemical, physical, and biological sciences are defined and discussed. The 21st century is shown to be the Age of Polymers.

INTRODUCTION

In terms of areas of research, polymer science and technology has expanded exponentially and transformed itself almost beyond recognition over the last two decades. This metamorphosis meant that the first IUPAC Polymer Conference on the Mission and Challenges of Polymer Science and Technology (IUPAC PC2002) was both timely and fruitful. The conference was conceived by one of the present authors (AA) and was held in Kyoto in December 2002 as part of the 50-year celebrations of the Society of Polymer Science, Japan. It was organized by the Science Council of Japan and the Society of Polymer Science, Japan, in collaboration with IUPAC's Macromolecular Division.

The scientific sessions of IUPAC PC2002 consisted of plenary lectures, scientific oral and poster sessions covering six areas, and a panel discussion (see Fig. 1) concluding the conference and discussing the role and activities of IUPAC's Macromolecular Division in the world polymer community. The six areas of the conference were Polymer Concepts in Chemistry, Physics, and Biology; Frontiers of Polymer Science; Advanced and Emerging Polymer Technologies; State of the Art in "Bio-Polymers"; Polymers and the Environment; and Commodity Polymers and the World Economy. The

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Fig. 1 Panel discussion in session at the IUPAC Strategic Polymer Conference (IUPAC PC2002). From left to right: Profs. Tatsuki Kitayama (Osaka University, Panel Secretary, Member, Subcommittee on Macromolecular Terminology, IUPAC Macromolecular Division), Kazuyuki Horie (Tokyo University of Agriculture and Technology, Panel Coordinator, Titular Member and Strategy Coordinator, IUPAC Macromolecular Division), Akihiro Abe (Tokyo Institute of Polytechnics, IUPAC Fellow), Gerhard Wegner (Max-Planck-Institut für Polymerforschung, Mainz), Kalle Levon (Polytechnic University, New York, Convenor of the next Strategic Polymer Conference, PC2005), Robert Stepto (UMIST and University of Manchester, President, IUPAC Macromolecular Division), Jung-Il Jin (Korea University, Vice-President, IUPAC Macromolecular Division), Mitsuo Sawamoto (Kyoto University, Task Group Leader of the IUPAC Macromolecular Division Project Strategic Study of World Polymer Science), Bob Gilbert (Sydney University, Past-President, IUPAC Macromolecular Division), and Dr. Michael Hess (Gerhard-Mercator-University, Duisburg, Chairman, IUPAC Macromolecular Division Subcommittee on Macromolecular Terminology).

progress in and challenges to polymer science and technology were reviewed and discussed by prominent plenary lecturers, whose papers are published in the present issue of *Pure and Applied Chemistry* [1–3]. In addition, most of the invited lectures of the conference will be published in a special volume of *Macromolecular Symposia* [4].

The present article highlights and summarizes, with a broad brush, the historical development of polymer science and technology and the recent advances that have occurred and are occurring in the subject. It highlights the mission and challenges for the future, particularly as reflected in the papers presented at the conference and in the conference's concluding panel discussion. The important role of IUPAC in defining and leading developments in polymer science and technology is also described.

STRUCTURE, BASES, AND DEVELOPMENT OF POLYMER SCIENCE AND TECHNOLOGY

Historical aspects [5]

Natural polymers have been used by man since prehistory and have been modified and processed empirically over many centuries for various applications, for example, textiles for clothing and papyrus.

Most of the early modifications that are still used today stem from developments in the 19th century or the beginning of the 20th century and relate to cellulose and natural rubber, for example, the mercerization of cotton by Mercer (1844), the production of cellulose nitrate (1845), cuprammonium rayon (1859), cellulose acetate (1869) and cellophane (1908), the production of a waterproof fabric using natural rubber by Macintosh (1823), and the cross-linking of natural rubber by Goodyear (1839).

The first, wholly synthetic polymer material, phenol-formaldehyde resin (Bakelite), was developed by Baakeland from 1905 to 1909. It was followed by urea-formaldehyde resins in the 1920s and polyester (alkyd) resins in the 1930s. Linear vinyl polymers were discovered early, poly(vinyl chloride) in 1872 and poly(methyl acrylate) in 1880, but were not produced commercially until much later, for example, poly(vinyl acetate) in 1920, poly(methyl acrylate) in 1927, and poly(vinyl chloride) in 1930. Many of the other conventional linear polymers of today formed by chain polymerization were developed in the 1930s to 1950s with something of a hiatus during World War II. The researches of Ziegler and Natta in 1953–1955 developing coordination catalysts for the polymerization of ethylene and propylene resulted in the award of a Nobel Prize (1963). The important advance was one of closer control of chain structure in terms of the minimization of branching and the control of tacticity. Significantly, the close control of chain structure is still important for the development of polymer materials of the future.

The initial developments of synthetic polycondensation and polyaddition polymers occurred from about 1928 to 1947. The work of Carothers [6] from 1928 to 1932 at the E. I. duPont and de Nemours company led to the controlled preparation of polyesters and polyamides. This was followed by the development of poly(ethylene terephthalate) (PET) by ICI in 1943 and that of polyurethanes from 1939 to 1947 by Bayer at Farbenfabriken Bayer [7].

Notwithstanding the preceding advances spanning the last 200 years or so, the macromolecular structure of polymers was not recognized until the landmark paper published by Staudinger [8] in 1920 and was not fully accepted until several years later. Prior to Staudinger's paper, macromolecular properties were thought to be achieved through the association of small-molecule entities, and cyclic structures were often proposed. In this respect, the pioneering work of Carothers on the formation of polyesters and polyamides was important in establishing the covalent nature of macromolecules. Staudinger was eventually awarded a Nobel Prize in 1953.

Structure and bases of polymer science and technology

Recognition of the macromolecular structure of polymers was key to enabling the development of polymer science and technology to occur on sound scientific and engineering bases. Modern polymer science is a blend of particular aspects of organic chemistry, physical chemistry, materials physics and statistical mathematics, with, to a lesser extent, some aspects of inorganic chemistry. This blend is exemplified in the work of Flory (Nobel Prize, 1974), who was instrumental in establishing the physical chemistry of flexible polymer chains in solution and in founding polymerization statistics, the bases of modern polymer science. In addition to many research publications, Flory published a classic textbook of polymer chemistry [9] and an important monograph on the statistical mechanics of chain molecules [10].

Polymer technology is even more multifarious, combining polymer science with aspects of chemical engineering, mechanical engineering, and rheology, encompassing, for example, reactor design for polymerization from monomers through blending, extrusion, injection molding, vacuum forming, reaction injection molding to the production and use of polymer colloids for drug delivery and adhesives. The interdisciplinary nature of polymer science and technology and their close interactions with more traditional disciplines is illustrated in Fig. 2.

One of the fascinations of polymer science and technology is the interplay of the various factors related to its constituent disciplines. For example, the mechanical properties of polymers depend closely on their chemical structure and on their molecular size or molar mass. The flow behaviors of polymer

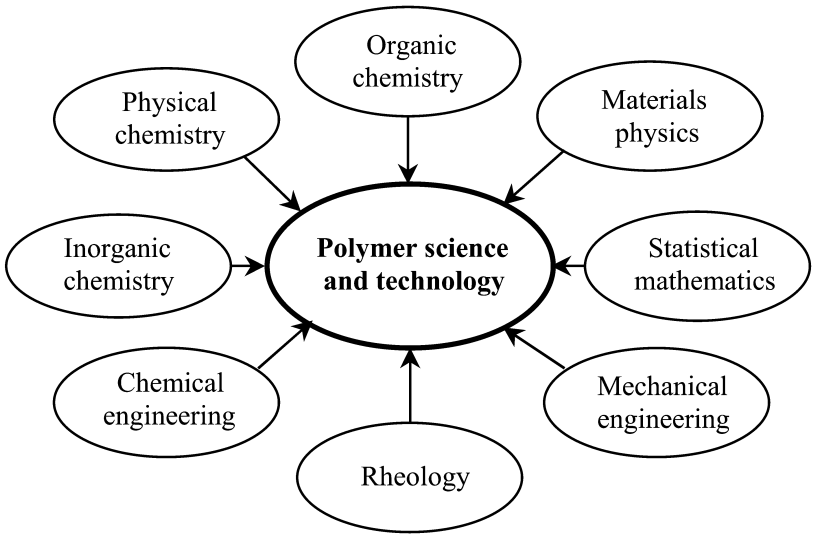

Fig. 2 Interdisciplinary nature of polymer science and technology.

melts and solutions and, hence, the design of processing methods and machinery are also intimately related to molecular size and structure. Significantly, by introducing scaling theory and the reptation model of polymer chain dynamics, de Gennes (Nobel Prize, 1991) enabled the thermodynamic and flow properties of polymer melts and concentrated solutions to be understood and interpreted in molecular terms [11].

The importance in polymer science and technology of the interplay of the various aspects related to its constituent disciplines arises because polymers are generally processed and used nearer the limits of their properties than are other structural materials. Therefore, there are more closely defined windows of conditions in which polymers display the desired properties. Molecular design and control are of paramount importance. For example, unlike brick or metal, polymers do not inherently have impact strengths that are one order of magnitude or more greater than those required in use. In addition, their desired performance often depends on molecular flexibility and extensibility, and these properties are intimately related to temperature, chain structure, molar mass, and molecular architecture (branched, linear, etc.). As polymer materials are usually organic substances, it is also important to ensure that they are chemically stable under the conditions of use.

Properties and applications of polymers in relation to their molecular structures

Polymers are the principal light and flexible materials in nature and human society. Compared with most inorganic structural materials, they are of low density ($\approx$1 g cm^{-3}). They are also the only type of homogeneous material that displays macroscopic, reversible elasticity.

The flexibility and elasticity of polymers is closely related to the rotational degrees of freedom that exist about the covalent skeletal bonds constituting the macromolecular chains and to the lengths of those chains. The net effect of many individual rotations along polymer chains is that those chains can move spatially in response to an external force. In addition to long, flexible macromolecular chains, reversible elasticity requires junction points at the ends of the chains to give an equilibrium network structure defining the spatial positions to which the junction points return after removal of the force. The junction points may be formed by interactions, entanglements, or chemical bonding between chains. Further, in the bulk, liquid state and in solution, polymers display both viscous and elastic properties that relate to the flexibility of their constituent macromolecules and the transient networks formed

by the mutual interactions and entanglements of those macromolecules. A well-known example of a type of polymeric viscoelastic liquid is non-drip (thixotropic) paint.

The flexibility of polymers notwithstanding, many polymer materials are designed to be rigid at their temperatures of use. By using stiffer (e.g., aromatic) chain structures, molecular flexibility can be suppressed. The glass–rubber transition temperature, T_g, is the important characteristic temperature with regard to suppression of flexibility. Below T_g, rotations about the skeletal bonds in a polymer chain may be neglected as significant degrees of freedom. The skeletal bonds then merely librate about equilibrium positions, and significant spatial movements of molecules cannot occur, resulting in rigid (glassy) materials. Engineering plastics, such as aromatic polycarbonate and polysulfone, show values T_g above 150 °C. Additionally, aromatic polyimides having long-term thermal stability above 300 °C have been used in space applications and also in the microelectronics industry as solder-resistant insulation materials.

The flexibility of polymers is also reduced if the chains carry a significant number of strongly interacting groups. Interactions between groups on different molecules enable ordered and, often, crystalline regions to form. The alignment of polymer chains and, hence, the degree of crystallinity can also be enhanced by extending or drawing the molten polymer during processing, as is done, for example, during fiber and, sometimes, film manufacture. Examples are polyamides, PET, and liquid-crystalline polyesters. Because the constituent macromolecules of amorphous polymer materials can never completely disentangle to become mutually aligned, completely crystalline polymers cannot be obtained. However, close control of the physical properties of polymers can be achieved by controlling the formation and concentration of ordered regions.

Network polymers can be made more rigid by increasing the concentration of junction points between normally flexible chains. For example, the vulcanization of natural rubber with about 1 % sulfur produces flexible elastomers, and about 30 % sulfur forms ebonite, a hard structural material.

An important, unique property of a flexible macromolecular network is that it cannot dissolve in liquids that are solvents for linear polymer chains of the same chemical structure as those that constitute the network. Because a network is essentially a single macromolecule of macroscopic extent, it can only swell in such solvents to form a gel, a soft solid whose structure is maintained by the junction points of the network holding together the polymer chains extended between them. Extremely large increases in volume, up to typically 1000 %, can occur. Polymer gels have many important applications, often associated with biology and medicine, for example, as soft contact lenses and superabsorbent swabs. In addition to such applications, Merrifield (Nobel Prize, 1984) proposed the use of cross-linked polymer gels in bead form for solid-state syntheses of proteins, facilitating rapid and important developments in biological science and technology over the last two decades.

Significant developments of functional polymers have also occurred over the last two decades. For example, although organic materials in general are insulators, electric conductivity was introduced into polymer films by Shirakawa, Heager, and MacDiarmid (Nobel Prize, 2000) by chemically doping polymers having conjugated backbones. Further significant developments have involved the introduction of photosensitive groups on polymer chains to bring about isomerization, cross-linking, ionization, chain cleavage, or other chemical reactions of polymers under photoirradiation. Such reactions are key processes in microlithography and holographic recording using photoresists and photosensitive polymers.

MISSION AND CHALLENGES OF POLYMER SCIENCE AND TECHNOLOGY

Background and overview

The polymer industry is one of major importance worldwide. The 21st century is the Age of Polymers. The volume of synthetic polymers produced is greater than the volume of steel. Furthermore, polymer consumptions of developed and developing countries increase roughly in proportion to their gross na-

tional products. Conventional plastics account for 88 % of the production of polymers, with 12 % being devoted to high-performance and specialist materials. It is this 12 % that is the principal focus of future research, leading to growth in volume, types of materials, and applications.

Until the mid-1980s, the main emphases of polymer research were linked directly with macromolecules, relating to their formation by polymerization and their physical, mechanical, and chemical properties, as summarized in the preceding sections. Since the mid-1980s, there has been a significant broadening of research areas and polymer science and technology is now interacting with many other modern scientific and technological disciplines. Furthermore, polymer science and technology is not just on the periphery but at the center of numerous exciting new developments. Such developments involve properties related principally to molecular structure, as in functional polymer materials displaying energy and charge transport and interactions (e.g., conduction, light emission, rapid-response electronic materials for information technology), and functional and structural polymer materials with properties related to molecular architecture (e.g., dendrimers for catalysts, rotaxanes for molecular switches, etc.). Also, research into polymer-based composite materials has increased greatly, covering, for example, materials formed by supramolecular assembly and polymer-inorganic composites.

Biological and biomedical applications of polymers, for example, for wound dressings, prostheses, drug delivery, nutrient delivery for plant growth, etc., have increased greatly. There have also been significant efforts made to develop environmentally friendly polymers, such as polymers from renewable resources and those that are biodegradable. The former, of course, reduces the dependence of polymer production on the availability of petrochemicals.

Another growth area of research is the improved control of the products of polymerizations through the use of new monomers and oligomers, catalysts, and polymerization mechanisms. Closer control of macromolecular chain structure, chain architecture, and molar mass, than has been obtainable hitherto using conventional polymerizations, is required to synthesize and optimize many new polymers, polymer materials, and applications.

Polymer science and technology is now so diverse and interwoven with other subjects that it is impossible to give a division of the subject into distinct, watertight areas. (Not that such a division is even desirable or necessary.) This diversity notwithstanding, the following sections give a categorization of the important and growing research areas that define broadly the future mission and challenge of polymer science and technology. Numerous examples of publications in the research areas can be found in ref. [4], the special volume of *Macromolecular Symposia* resulting from IUPAC PC2002.

Polymer concepts from chemistry, physics, and biology

As discussed in preceding sections, polymer science and technology has its foundations in flexible polymers and in elastic and thermoplastic polymeric materials. The traditional, basic molecular concepts of polymer science can be summarized as being based on polymer chains with single covalent backbone bonds, the flexibilities of those chains and average properties of distributions of molecular species. However, developments in biology and physics as well as the chemistry of small molecules are causing the introduction of new concepts into polymer science, for example, macromolecules with shape persistence in contrast to flexibility, precision polymerizations leading to properties defined by single polymer species rather than distributions of species, and polymers with weak interactions or conjugated bonds in addition to polymers with single covalent bonds.

In summary, we have now moved into a new era, “from simple polymers to more sophisticated (polymer-based) systems”. The development is a progression into the 21st century of the title of the book *From Small Organic Molecules to Large* [12], dedicated to the late H. F. Mark, who lived fully in the 20th century. The importance of polymer science and technology is expected to grow even further. As illustrated in Fig. 2, it already interacts with most areas of chemistry, and new developments are expected, especially involving life sciences and materials physics.

Frontiers in polymer chemistry and physical properties

Studies of polymer syntheses continue to play a major role in polymer research. The missions and challenges in the controlled syntheses of polymers and polymerizations, as exemplified by the papers of IUPAC PC2002, are summarized in Fig. 3, while the missions and challenges in new molecular architectures are summarized in Fig. 4. The development of control of the chain growth and termination reactions in macromolecular syntheses provides opportunities for reducing the stochastic nature of polymerizations and obtaining precisely defined products. In the design of supramolecular architectures, the use of weak interactions, often based on hydrogen bonding, both intramolecular and intermolecular, will remain a key factor. New molecular and supramolecular assemblies, for molecular recognition, on/off switching, chiral sensing, and other purposes are being proposed, based on hydrogen bonding, dendrimers, rotaxanes, and catenanes.

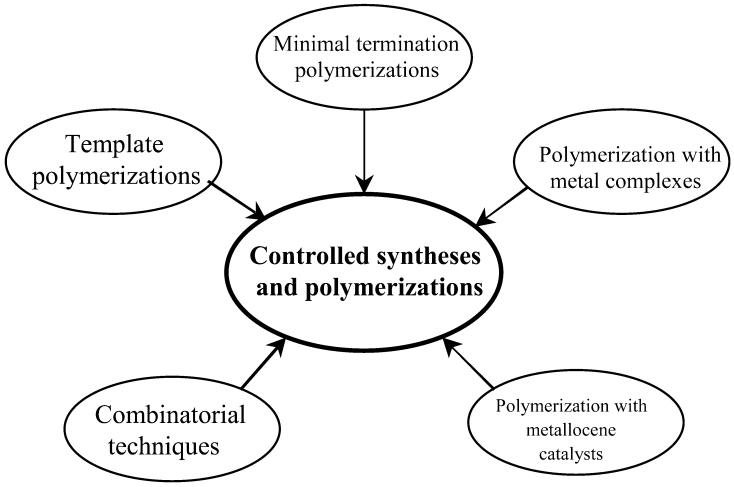

Fig. 3 Developments in controlled syntheses of polymers and polymerizations.

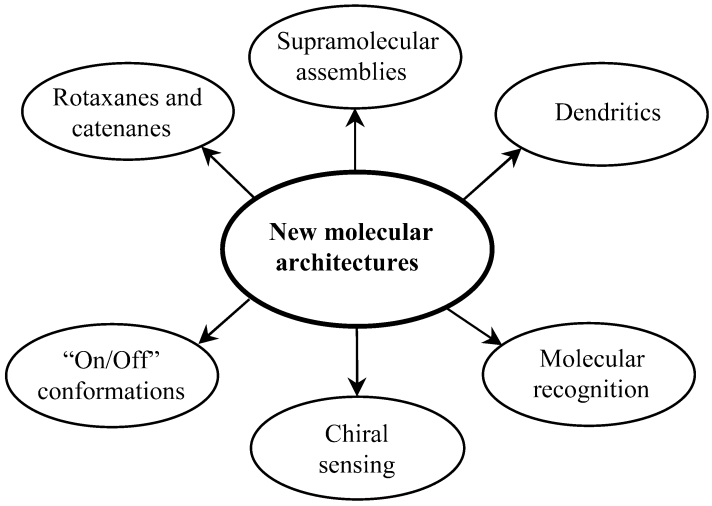

Fig. 4 New molecular architectures.

Polymer materials for energy and charge transport and interactions in polymers (Fig. 5) are areas of growing importance. One challenge is to understand the nature of electronic excitations, charge-carrier production and transport and the link between nanoscopic and macroscopic phenomena. Challenges, related to a wide range of systems and applications, also occur in the control and design of polymer-based structural and functional materials and processes (Fig. 6). The methodologies to investigate the structure and dynamics of such complex systems have not grown at the same rate as the numbers of reports of novel developments. NMR methods and scanning probing microscopy methods (AFM, near-field optics, etc.) play important roles and need to be developed further. In addition, further progress in the modeling of the relations between molecular, nanoscopic, and macroscopic structures and properties is needed in order to understand and predict the limits of performance that can be attained by polymers, particularly those of commercial interest.

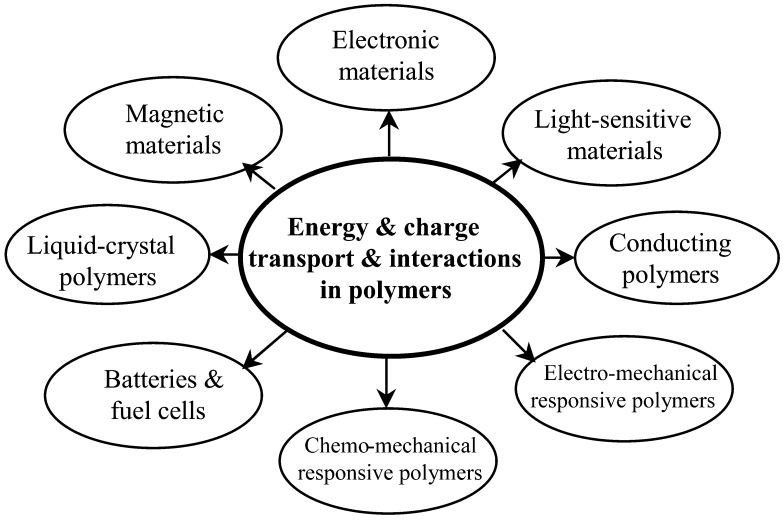

Fig. 5 Applications of energy and charge transport and interactions in polymers.

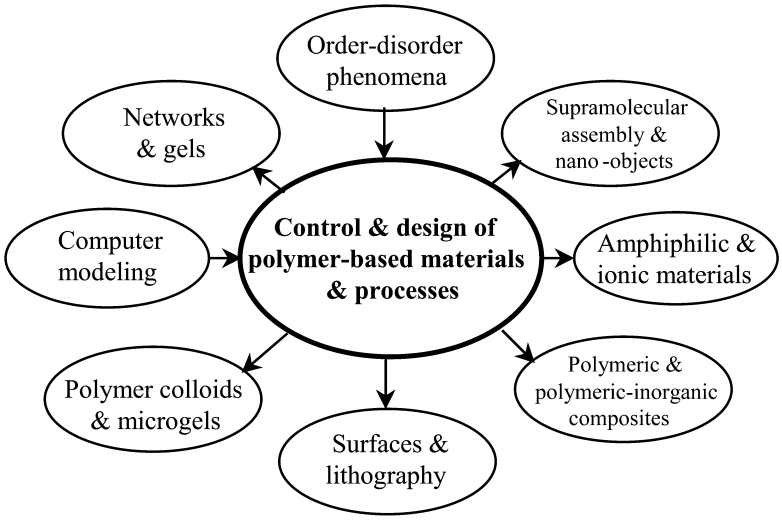

Fig. 6 Developments in the control and design of polymer-based materials and processes.

Biological, biomedical, and environmental applications and interactions of polymers

A number of important challenges in these areas relate to the design of materials for biomedical applications and diagnostics (Fig. 7). Modified proteins, nucleic acids, and other natural materials serve as novel functional molecules in various applications, including nanotechnology, and polysaccharides are being applied to cell-sheet engineering. Supramolecular assembly, biomimetic architecture, molecular recognition, and molecular machines and motors are being used to derive biological functional materials from chemical and molecular starting points.

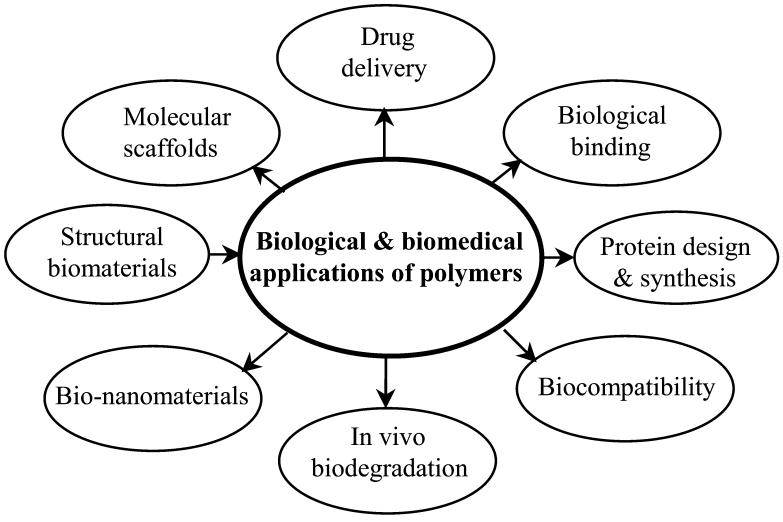

Fig. 7 Biological and biomedical applications of polymers.

Research into and development of biologically based, recyclable, and environmentally degradable polymers have become important for the sustainable coexistence of polymeric materials and the environment (Fig. 8). In this context, thermoplastic starch and polyactide (PLA) are two important new products based on renewable resources to be commercialized by the plastics industry. Also, the devel-

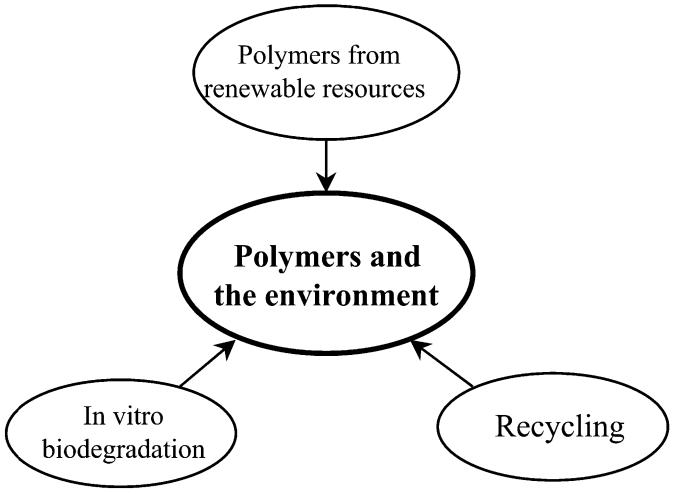

Fig. 8 Developments regarding polymers and the environment.

opment of biodegradation, environmental degradation, and recycling technologies of commercially available polymers such as PET, nylons, polyurethanes, elastomers, and fiber-reinforced plastics are challenges that now face the world polymer community.

LEADERSHIP ROLE OF IUPAC'S MACROMOLECULAR DIVISION

Status and activities of the Macromolecular Division

IUPAC is a global body with a mission to advance the chemical sciences worldwide and to contribute to the application of chemistry in the service of mankind. The activities of IUPAC are funded principally through financial support from its 44 National Adhering Organizations that are in turn funded by national governments.

The Macromolecular Division is responsible for the activities of IUPAC in the areas of polymer science and technology. The Division is one of the most active within IUPAC. It seeks to define and respond to world needs and to improve communication and learning in its subject area. It has over 300 scientists involved in 55 current projects and is very conscious that its success and continued activity depend on the goodwill and dedication of individuals, whose efforts and time are given without financial reward.

The Division runs projects in three main areas—characterization, terminology and nomenclature, and developing polymer materials systems. The Division also sponsors conferences and educational projects and courses, worldwide. The levels of activity and output are high and topics of present-day interest and importance are addressed. Examples of publications resulting from recent projects are given in refs. [13–16]. Industry is closely involved in many of the projects and this assures the Division's relevance for the future and its level of activity. The industrial involvement in terms of time and resources represents a very large financial input in kind.

The Division's program of conference sponsorship is second to none. About 12 conferences are sponsored annually and almost all of the conferences result in journal or book publications. Currently, more than 50 % of the volumes of *Macromolecular Symposia* come from IUPAC-sponsored conferences approved via the Macromolecular Division.

The emphasis of the educational projects and courses is to spread polymer education into economically disadvantaged countries. In the last year, the Macromolecular Division has supported a project based in Moscow aimed at distance (Web site) learning, a school and workshop, joint with UNESCO, in South Africa, and postgraduate courses based in Prague and in Denton, USA.

The way forward with IUPAC

The Macromolecular Division is the only worldwide organization leading polymer science and technology. It funds projects and sponsors conferences of relevance to the future development and application of polymers for the benefit of the world community. It also spreads knowledge about polymers, particularly to students from economically disadvantaged countries, through the educational projects and courses that it sponsors.

Every two years, the Macromolecular Division sponsors and helps to organize the World Polymer Congress, the principal polymer conference in the international calendar that covers all topics of present-day and future importance. The Congress in 2002 was held in Beijing, that in 2004 will be held in Paris, and in 2006 the Congress will be held in Rio de Janeiro.

Importantly, the Macromolecular Division has initiated Strategic Conferences on the Mission and Challenges of Polymer Science and Technology. As stated at the beginning of this article, the first one was held in Kyoto, in December 2002, and the next one will be held in New York in 2005 (see caption to Fig. 1).

Over the next three years, the Division is also undertaking a Strategic Study of World Polymer Science Organizations, providing an overview and analysis of the trends in contemporary polymer science and technology around the world. The results will enable the Division to formulate future strategies and activities in order to guide and help the world polymer community. By working through world polymer science organizations, the Division will be able to formulate an objective, systematic, and updated view of the trends in polymer science and technology and, hence, perceive and define the mission, challenges, and strategies for the future. The results of the study will be publicized widely, and will be presented at forthcoming World Polymer Congresses and Strategic Polymer Conferences.

Through its projects, conferences, and educational courses and now through its strategic conferences and its strategic study, the Macromolecular Division seeks to play a leading role in defining and guiding the worldwide future of polymer science and technology. Detailed information on publications, current projects, future conferences, courses, and the scientists and technologists involved can be obtained from the Division Web site <www.iupac.org/divisions/IV>.

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