Present and Future Directions of Basic Research on Polymeric Materials

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ABSTRACT: Polymer science is in the midst of profound changes in direction. Historically, the foundation of polymer science has been primarily chemistry, *i.e.*, the preparation of polymers and physical-chemical studies of their properties. At the present time, the frontiers of the science are being pushed increasingly toward condensed-matter physics and materials science. One reason for this trend is, undoubtedly, the intellectual nourishment that polymer scientists are finding in these fertile fields which, themselves, are undergoing some great changes of their own. Another, of perhaps even greater potential importance, is the discovery by many scientists with little prior interest in polymers that these materials offer an intellectually challenging area of research. A still further impetus comes from the demands of dynamic "high-technology" industries for new materials with new properties. Eventually, bridges will also be built to the biological sciences. All of these changes are occurring at a time when the ever-increasing power of the instrumentation and computers available to the researcher is providing new insights. Together, these forces are reshaping the way in which basic research on polymeric materials will be conducted in the future.

KEY WORDS Polymer Science / Chemistry / Physics / Materials Science /
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Instrumentation / High-Technology Industries /

This 2nd SPSJ International Polymer Conference has as its theme "Specialty Polymers for High Performance." It is designed to cover in depth certain topics of great interest to contemporary polymer science, namely high-performance polymers, advanced composites, conductive polymers, the photochemistry of polymers, and polymers for high-technology applications. Each of the papers represents a significant, tangible advance in the field. Most academic basic research, in Japan as well as in the United States, is carried out in this way: by *individual researchers*, or small groups of researchers (*e.g.*, a professor with several students and postdoctoral fellows). The publications that result from such an effort generally constitute small, but nevertheless very significant, steps in the forward march of science.

Each of these individual efforts can be further grouped into *subareas of science*. In the NSF Polymers Program, the subareas of basic polymer science that we are funding at present are listed in Table I, where the percentage of the Program's total funding allocated to each of these subareas in 1986 is also shown. The Engineering Directorate and other parts of NSF provide additional funding for subareas of polymer research not covered by the Polymers Program.

This paper presents the author's view of the general directions in which the field of polymer science *as a whole* is moving, and of the forces that are changing the way polymer science is being carried out. It does not present in any detail the diverse research being carried out by the thousands of polymer scientists throughout the world (among which are over seven

Table I. Subareas of polymer science in NSF Polymers Program (1986)

	%
Morphology and blends	23.8
Synthesis, reactions	23.5
Solution properties	17.9
Molecular dynamics	10.3
Characterization	7.7
Mechanical properties and composites	6.6
Electro-optical properties	4.7
Surfaces and interfaces	4.5
Others	1.0
	100.0

hundred professors in American universities).

Before we begin this journey into the future, it is instructive to learn from the past. The wonderful book by Professor Herbert Morawetz, *Polymers: The Origins and Growth of a Science*,¹ traces the intellectual roots and development of our science. Contemporary polymer science grew out of chemistry: all the great pioneers—Staudinger, Mark, Sakurada, Carothers, Champetier, Flory, Kargin, Marvel, Melville, and others—were trained as chemists. Some of these (like Marvel) were mainly interested in synthesis, others (like Mark) primarily in physical properties, and still others (like Flory) primarily in theory. The scope of most, however, encompassed *several* of these aspects, *e.g.*, synthesis as well as physical properties of the resulting polymers. The work of the polymer chemist thus emerged as fitting *neither* purely organic chemistry, *nor* purely physical chemistry, *nor* purely any of the other traditional subdivisions of chemistry. [Some people have even viewed it, incorrectly, as an applied art.] This key distinction makes it difficult—even a half-century after Staudinger's work—for polymer chemists to fit easily into traditional chemistry departments in universities, and causes an undesirable isolation of polymer chemistry from the remainder of chemistry. This point was made with great emphasis in the report issued by the US Academy of Sciences in 1981.²

Figure 1. Maximum tenacity achieved in experimental fibers of carbon and polyethylene as a function of time. Courtesy Paul Smith (du Pont).

It should be noted that physicists have also, until recently, shunned polymers, but probably for different reasons: their complexity, and the attraction of biophysics and molecular biology.

But if polymer science has not really achieved full acceptance in some quarters, it has nevertheless immensely flourished. The level of polymer science has been remarkably high, and has had a major impact on science and technology as a whole. In the past few years, polymer scientists have reported such important achievements as synthetic self-assembling systems with remarkable morphologies,³ “living” cationic polymerization,^{4,5} polymers approaching the theoretical limit in strength⁶ (see Figure 1), and the direct measurement of adsorptive forces on inorganic substrates.⁷ These are but a few examples of the vigor of contemporary polymer science (taken primarily from subareas of the field not covered at this Conference). The creation and development of specialized departments of polymer science in several universities; the large number of scientific journals, books, meetings and symposia; and the rapidly increasing membership in our scientific socie-

ties (e.g., 8241 members in 1985 vs. 4274 in 1975 for the Polymer Division of the American Chemical Society) are still other undeniable signs of an astonishing vitality.

Yet, in the midst of this vitality—nourished by the inventiveness and energy of polymer scientists—there are emerging signs that polymer science, as we know it today, is also being reshaped by powerful forces that are essentially external to it:

the dramatic advances being made in other fields of science;

the enormous power of the new instrumentation;

the demands for materials by the “high-technology” industries.

Let us examine each of these.

THE IMPACT OF ADVANCES IN OTHER FIELDS OF SCIENCE

We are in the midst of one of the most dynamic periods in the history of science; for example, the number of scientists active today is far greater than at any other time in history, and we are witnessing an astonishing growth in the acquisition of new knowledge. (It has been

estimated that there are some 750 000 scientists and engineers in the United States working in research and development.) Inevitably, the advances in other fields of science are leaving their impact on polymer science; this is particularly the case with physics.

Physics

Physicists, who traditionally have played only a secondary role in polymer science, are becoming increasingly active as sources of new ideas and deeper insight into polymer problems as well as active participants, themselves. Table II is a compilation of new concepts and techniques that physicists are contributing to polymer science.⁸

There can be no question that de Gennes' book *Scaling Concepts in Polymer Physics*⁹ is the most influential since Flory's *Principles of Polymer Chemistry*.¹⁰ De Gennes' ideas originate directly from the mainstream of physics. The same may be said for the profound advances in conductive polymers by Heeger, Schrieffer and others, and the fundamental concepts of the behavior of macromolecules being contributed by Edwards and Doi.⁸ One of the most exciting aspects of current research

Table II. Some ideas from (and to) physics

Physics		Polymer science
	At present	
Magnetism	} →	Polymer behavior
Renormalization group theory		Properties of concentrated solutions
Scaling concepts		Self-diffusion
Percolation		Gelation
Solitons		Conductivity in polymers
Low dimensionality		Polymer conformation
Low dimensionality	→	Langmuir–Blodgett films
	In future	
Low-temperature physics	→	Behavior near 0 K
Ultrahigh pressures	→	Phase transitions
Superconductivity	→	Polymeric superconductors
Superlattices	→	New designed morphologies
Epitaxy	→	Layered polymers
Fractals	→	“Treeing” in plastics
New theories	↔	Model polymers
Molecular electronics	←	Polymer structure and morphology

is the growing interplay of theoretical physics with experimental polymer science, and the greater rigor and predictive power resulting from this confrontation.

There are already over forty physics professors in American universities working on polymers. In my opinion, the physicists' role will increase still further in the future, as their ideas become better understood by polymer scientists and even more physicists take up the difficult challenges of complex, polymeric systems.

Chemistry

There is a perceptible change among American chemists in their attitude toward polymer science. Some "traditional" chemists are already seeking ways to apply their special expertise to the study of polymers, and others are taking the first, tentative steps in that direction.^{2,11} At the same time, several prestigious universities are now seeking to expand, or begin, teaching and research in polymers. The National Science Foundation is nurturing this trend by paying special at-

tention to the borderline of chemistry and polymer science; we call this interface *materials chemistry*.

Table III gives examples of what the traditional subfields of chemistry are contributing to polymer chemistry. A notable recent event is the synthesis of the highly branched polymers known as dendritic (or starburst) polymers¹² or arborols.¹³ The table illustrates that the flow of ideas also goes from polymer science to chemistry!

Biological Sciences

From the beginning, there has been a clear link between the study of polymers—synthetic macromolecules—and biological macromolecules; *e.g.*, cellulose, natural rubber, and proteins were among the first macromolecules studied.¹ However, as molecular biology blossomed and became ever more specialized, that link weakened considerably so that, today, the two fields are quite separate.

Table IV shows some of the new insights that polymer scientists have obtained from the biologists. Here, the interactions are still

Table III. Some ideas from (and to) chemistry

Chemistry		Polymer science
	At present	
Organic chemistry	→	Group-transfer polymerization, new reactions at surfaces, crown ether polymers
Organic chemistry	←	Polymeric reagents
Organometallic chemistry	}	{ Olefin metathesis mechanism (SN) _x , polyphosphazenes
Inorganic chemistry		
Physical chemistry	}	{ Quasi-elastic light scattering Excimer fluorescence
Analytical chemistry		
Solid-state chemistry	→	"Stacked" conductive polymers, liquid-crystal behavior
Phase-transfer catalysis	←	Interfacial polymerization
	In future	
Organic chemistry	→	New types of polymers: "arborols," helical polymetalloenes, etc.
Physical chemistry	→	More efficient photochemical systems; kinetics and dynamics; chemistry under extreme conditions
Organometallic chemistry	→	Catalytic polymers
Electrochemistry	→	With monomers or polymers
Solid-state chemistry	→	Polymeric ionic conductors
Solid-state chemistry	←	Polymeric liquid crystals
Atmospheric chemistry	→	Mechanisms of gas-phase polymerization

Table IV. Some ideas from (and to) the biological sciences

Biological sciences		Polymer science
Molecular biology	→	Helicity, steric specificity
Enzymes structure	→	Synthetic enzymes, catalysts, "biomimetic" polymers
Base pairing	→	Specific functional sites in polymers
Vesicles, liposomes	→	Polymeric analogs
Aggregation phenomena	→	Gelation
Primary structure	→	Periodic copolymers with <i>many</i> types of monomeric units
Biotechnology	→	Monomers, polymers
Merrified synthesis	←	Ion-exchange resins
Biological materials	←	Materials science

Table V. Some ideas from (and to) metallurgy and ceramics science

Metallurgy and ceramics science		Polymer science
Phase transformations	→	Spinodal decomposition in polymers
Martensitic transformation	→	Epitaxial polymerization
Fracture, tribology	→	Mechanical behavior of polymers, incl. crazing
Defects: disclinations, grain boundaries	→	Interfaces in multicomponent polymers
Electron microscopy	→	Application to polymers
Surface analysis	→	Application to polymers
Epitaxy	→	Epitaxial growth in polymers
Positron annihilation	→	Voids and free volume
Glasses, amorphous metals	←	Amorphous polymers
Free volume	←	Physical aging
Ceramics synthesis	←	Polymeric precursors
Sol-gel process	←	Polycondensation
Modification of glass surfaces; inorganic-matrix composites	←	Composites

tenuous, but a few far-sighted scientists are beginning to venture into the interface between the two fields. As we strive to emulate biological systems by building higher specificity in function into synthetic polymers, by seeking yet more effective ways of controlling the steric structure of polymers, and by searching for new methods of controlling sequences of different monomeric units (beyond the three that seem to be the limit at this time), a new rapprochement of the biological sciences and polymer science seems inevitable. The emerging recognition that biological materials (*e.g.*, muscle, bone, organs) are amenable to study by the methods of materials science will aid this process.

Metallurgy and Ceramics Science

The fields of metallurgy and ceramics science, both based on ancient industries, are in a state of vigorous rejuvenation. Polymer scientists are learning much from these fields, in such important areas as phase separations and transformations, fracture and fatigue behavior, tribology, the effect of grain boundaries and defects on properties, and the effective use of electron microscopy and surface-analytical techniques, which are far more advanced in these disciplines than in polymer science.⁸ Table V shows that the movement of ideas to and from polymer science is about equal.

Table VI. Examples of modern instrumentation for polymer research
(in approximately decreasing cost)

Instrument	Typical application
(Very expensive)	
SANS	Molec. arrangement in crystals, networks
Synchrotron radiation	Photolithography
● Rutherford backscattering	Crazing
● EXAFS	Ionomers
Supercomputer	Previously unfeasible calculations
30 T magnets	NMR, liquid crystals
(Expensive)	
STEM, TEM, SEM	Studies at low dimensions
Solid-state NMR	Macromolecular dynamics, networks
XPS, etc.	Surface composition
SAXS	Phase separations, crazing
Cloud chambers	Kinetics of gas-phase polymerization
Ultrafast spectroscopies	Macromolecular dynamics
(Moderately expensive)	
LAM-Raman spectroscopy	Defects in crystals
FTIR	Surface analysis, hydrogen bonding, etc.
Lasers	Photochemistry
QELS	Diffusion in solutions, amorphous polymers
Israelachvili apparatus	Adsorption forces
Microcomputer	Faster calculations
Minicomputer	Operation of lab apparatus

THE IMPACT OF NEW INSTRUMENTATION

Much of modern science, including of course research on polymeric materials, is instrument-driven and perhaps instrument-limited.⁸ The new instruments are both more powerful and allow measurements of a kind that was previously unfeasible. Access to these instruments is an absolutely essential requirement for research at the frontier of science. Because of their size, cost, and complexity, some instruments can be located only in a few, nationally maintained laboratories to which the scientists must travel. That is the case for the first of the three groups in Table VI, which divides instruments by approximate cost. All large instruments share the characteristic that they require a specialist for their optimal operation; thus, polymer researchers are becoming increasingly dependent on these specialists for their research.

Polymer science has been enormously aided by many new instruments. Let me cite a recent example. Using a Class VI computer, Suter was able to achieve the first calculation of bulk properties of a polymer (atactic polypropylene) from basic principles of atomistic behavior, rotational isomeric state theory, and long-range interactions.¹⁴ This extraordinary feat would not have been possible, even using a supercomputer, were it not for stagewise minimization to reduce the immense number of calculations. The results of these calculations agree remarkably with experimentally determined values of several properties of the bulk polymer.

THE DEMANDS OF "HIGH-TECHNOLOGY" INDUSTRIES

Polymers are increasingly being used in many of the most demanding industrial applications.¹⁵ They have several, well-recognized

Table VII. Examples of polymeric materials used in "high-technology" applications

Polymers	Applications
Photodegradable polymers	Photoresists
Photopolymerizable systems	Photoresists
Conductive polymers, incl. ionic conductors	Batteries
Magnetic polymers	Recording media
Ferroelectric polymers	Transducers
Structural composites	Space vehicles, aircraft, flywheels, automobiles
Fibers	
Matrix materials	
Liquid-crystalline polymers	Structural materials; nonlinear optics
Thin films	Electronic devices; membranes
Polyimides	Electronic packaging
Adhesives	Rapid assembly
Biocompatible polymers	Prostheses, drug carriers, drugs
Oligomers	Functional polymers
Polymeric coupling agents	Composites

advantages: a broad range of chemical structures coupled with increasingly precise control of the molecular architecture and morphology, ease of fabrication, and great versatility in the physical properties that are possible. A few examples of "high-technology" applications are given in Table VII; this important subject is dealt with in greater detail in the preceding paper,¹⁶ and in many others at this Conference.

The interest in polymers for "high-technology" applications is widespread because it is tied directly to the future economic competitiveness of industries. In the United States, the NSF has provided several mechanisms for aiding collaborative research between universities and industrial organizations, including small businesses. Similar objectives are being pursued—although possibly by different mechanisms—in Japan (through the ERATO Fine Polymers Project directed by Professor Ogata), in France, Italy, and several other countries.

Research to meet the specialized needs of "high-technology industries" demands the utmost versatility in synthesis, as well as a profound understanding of such other sciences as physics, materials behavior, mechanics, biology, etc. Another important distinction is

that polymers are simply *one* of many materials available to meet a given functional requirement. Thus, familiarity with a broad range of materials, whether they be polymeric or not, is essential.

THE FUTURE OF POLYMER SCIENCE IN UNIVERSITIES

It now remains for us to consider some of the anticipated consequences of these trends. In the author's view, they will be significant and will alter, in a profound way, what is now considered to be polymer science. The professional environment of the academic polymer scientist will also be affected.

The growing influence of the condensed-matter physicists is expected to drive polymer research increasingly closer to the field of physics. Similarly, the increasing involvement of talented chemists *without* prior history of contributing to the field of polymers is going to shift polymer science much closer to the mainstream of chemistry. A comparable statement can also be made for the growing commonality between polymer science and the other materials sciences, namely metallurgy and ceramics science. But the movement will not be one-way: many of the newcomers gravi-

Figure 2. Convergence of several sciences to create the new discipline *materials science*.

tating toward polymer research are finding that success requires knowledge and insight of a kind that their prior background in physics, chemistry, or metallurgy does not provide. And, as has been shown above, polymer science has much to contribute to other sciences.

As the sciences dealing with materials get increasingly intermingled and mutually dependent, a new blend is emerging at their confluence: it is a fusion of polymer science and engineering, metallurgy and ceramics science, with components of chemistry and physics, mechanics, rheology, and, eventually, biology. That composite is the new discipline of *materials science*! This blending is illustrated in Figure 2. One consequence of this trend should be that few, if any, new departments of polymer science will be created in major American universities—but there should be many departments of materials science.

Because the science will be changing, we can expect that academic and professional organizations, and the way scientists carry out their research, will also be profoundly altered. Few individual scientists will be able to deal, alone, with the widening scope of materials research and the ever-increasing size, cost, and complexity of the powerful new instruments. Most will find that they lack the specialized knowledge to make a broad contribution to the diverse and difficult research on new high-

performance materials. Many university scientists (but by no means all) will conclude that *multidisciplinary groups* are the best way to make progress in materials research—a path already encouraged by the government agencies funding academic research.

The polymer scientist will then become *one* specialist in a team comprised of *several* specialists working, in common, on broad problems. This cooperative mode of research, well known in industry, is already seen in American universities in the Materials Research Laboratories, Materials Research Groups, and Engineering Research Centers—all funded by the National Science Foundation. Table VIII shows a typical budget for a Materials Research Laboratory, compared with the budget for a NSF grant to a single senior investigator. Table IX illustrates the scope of a major research theme at such a laboratory; a variety of techniques is being applied to both scientific and technological issues.

In this multidisciplinary environment, the ties of the scientist to his original discipline will inevitably be weakened. This trend will force universities and scientific organizations to adapt or find themselves increasingly obsolete.

The Critical Role of Synthesis. Finally, the increasingly critical role of the synthesis specialist should be noted. In the new organization of research that has been described, he will be called upon not only to find still better

Table VIII. Typical NSF budget for different kinds of research groups, in k\$

Individual investigator		Multidisciplinary group
40	Salaries	950
1 professor, 2 students		11 professors, 43 students, 2 postdocs, 16 technicians, 8 secretaries
5	Materials	320
3	Travel, misc.	95
9	Equipment	675
23	Overhead	960
80	Total	3000

Table IX. Scope of a typical major research theme at a NSF-funded Materials Research Laboratory

Polymer interfaces
<u>Scientific issues</u>
Preparation of novel interfaces
Dynamics of chains on surfaces and in confined spaces
Conformations of constrained chains
Thermodynamics of interfaces
Interfacial electronic states
Dielectric behavior
<u>Technological issues</u>
Adhesion
Separations
Fabrication of electronic devices
Remote sensing
Colloid stability
<u>Techniques</u>
Theory
Synthesis
Spectroscopy
Microscopy
Electrophoresis
Measurements of electronic and dielectric properties
Calorimetry

ways of controlling the molecular architecture, but also to use his utmost ingenuity to produce new functional materials—for a major theme of future research will be the discovery of *new* phenomena and *new* properties through the study of *new* polymeric materials. An additional, and increasingly crucial, role will be to prepare special materials needed by the physicist or the engineer in the team. This is illustrated in Figure 3. Both of these functions

Figure 3. Expanded role for synthesis.

—one more creative, the other more supportive— should bring forth a renaissance of organic polymer chemistry.

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