Polymer Breakout Report

Identification of Grand Challenges

Breakout Polymers

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- Speakers:

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- Participants: Same

State of the Art in Polymer Science & Engineering

- Polymers are never pure; they often consist of distributions (molecular weight, stereoregularity, composition, crystallinity, branching, charge).
- The possibilities for discovery are extraordinary – every molecule is different
- Polymers are always changing and rarely at equilibrium. Spectrum of relaxation times spans many decades of frequency.
- Properties can deteriorate over time.
- Polymers can exhibit intricate 3D morphologies that sometimes approach complexity of biology. Characterization of such morphologies and the corresponding properties is exceedingly difficult.
- A few polymers (e.g. polyethylene) dominate market and applications. Specific properties are “tuned” by blending such polymers and using additives. Formulations are widely used and not well understood
- Polymers in complex systems are not understood.
- Data for specific polymers that include distribution information, equilibrium properties, dynamic (transport) properties and rheological behavior are not available.

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- Polymers exhibit many universal characteristics, but models capable of predicting properties (structure, phase behavior, dynamics, and rheology) are not available. Mesoscale models that link the microscopic structure to macroscopic behavior are beginning to emerge but are limited to simplest of materials.
- We cannot predict the behavior of mixtures on the basis of pure component properties. Potentials are not readily available. Rheology difficult to predict.
- These deficiencies also apply to polymer colloids.
- Processing changes properties and is not fully understood.
- Ability to synthesize specific sequences/architectures is limited. Industrial materials design and processing are Edisonian.
- We cannot describe the behavior of charged polymers.
- Bench-top methods for characterization of all properties (e.g. branching) are often ambiguous. More definitive methods (e.g. scattering) are not widely available or well understood.
- Data sharing is limited.

Opportunities and Usefulness

(What do you think would be the gains, with respect to materials discovery and deployment, of adapting an MGI approach in the XYZ industry? What are the most promising opportunities? What are the least promising opportunities?)

Opportunities and Usefulness

- Lightweight, high-performance, inexpensive materials in a wider array of applications
- Better materials for separations, including in water management, gas technology, energy
- Multifunctional, tough materials for sensing, display technologies, electronic devices, biomedical applications, packaging
- Better batteries; lighter weight, higher energy density, long-term performance
- Solutions, complex formulations, colloidal systems, multilayer materials for innovative applications

Technical Challenges and Gaps

(What are the primary technical challenges and gaps preventing application of integrated theory/modeling and synthesis/characterization towards accelerated development/deployment in your industry?)

- Tools:
- Infrastructure:
- Culture:

Overall Challenge

Establish an MGI-based approach to design, model, synthesize, and characterize complex polymeric materials with target functionality in an extraordinarily large parameter space

- → Enable Materials Discovery – extraordinarily large palette of building blocks
- → Enable materials by design in a large parameter space
- → Enable superior performance – aerospace, energy, transport, protection, electronics, infrastructure , healthcare
- → Accelerate development and deployment
- → Identify failure modes in sensitive applications
- → Predict long time behavior during exposure to demanding conditions (stress, strain, temperature, pH, etc.)

Grand Challenge 1:

Mesoscale Models of Equilibrium and Non-Equilibrium Structure and Morphology, Properties (including rheology), and Behavior During Processing

If polymer scientists could predict and control the equilibrium and non-equilibrium behavior, including rheology, of polymers of arbitrary structure, sequence, charge distribution, morphology and their blends, then materials process engineers could:

Discover unknown materials

- Design more effective processes for demanding high-tech applications (roll-to-roll printed electronics, nanolithography, medical implants)
- Formulate multicomponent systems on-demand for specific applications
- Design materials that approach the complexity of biological systems but surpass their performance

Grand Challenge 2:

Design the hierarchical structure of polymeric materials for functionality

If polymer scientists could predict, design and then synthesize new materials that have controlled architectures, multi-unit (>>3) sequences, mesoscale morphology and target functionality from a large pool of building blocks, then polymer scientists and engineers could:

- Usher in an era of bottom-up synthesis and assembly by design
- Expand the uses of polymeric materials
- Enable unknown applications thru multi-functional materials with heterogeneous sequence

Grand Challenge 3:

Curate and make easily available comprehensive data sets and samples

If polymer scientists could identify the structure, sequence, thermodynamic properties, transport properties, rheological and other properties that constitute a complete data set, generate such data for a variety of materials, and make samples available, then polymer scientists and engineers could:

- Understand material properties in complex polymer structures and distributions
- Accelerate material down selection for industrial applications
- Develop correlations for materials design
- Develop data base for model validation
- Prepare formulations on the basis of actual data

Grand Challenge 4:

Characterization and interpretation of 3D structure and dynamics in real time

If polymer scientists could determine from combined experimentation and modeling , in real time, the structure and dynamics of polymers simultaneously at length scales from 1 nm to 100 μm and time scales from nanoseconds to minutes, we could

- Accelerate the screening of materials from years to days
- Better understanding of interfaces would enable better materials integration
- Better insights at earlier stages of development

Grand Challenge 5:
Identify, model, predict and control evolution of properties over long time scales

If polymer scientists could identify decay/evolution mechanisms and quantify the corresponding property changes in a material, then materials process engineers could:

- Reduce testing time and costs (from current time of several years)
- Improve performance and sustainability
- Control life time
- Enable deployment of new light-weight materials in high-performance applications (including aerospace, transportation, energy, separations, biomedical, packaging)

Grand Challenge 6:

Computer-enabled identification of responsive polymers designed for extreme environments

If polymer scientists could computationally accelerate the identification of strategies to improve the performance of polymers in extreme environments (pressure, temperature, radiation, pH, etc.) then materials process engineers could:

- Use multifunctional polymers for new applications
- Speed up deployment of new inexpensive materials in demanding applications
- Expand the application space of lightweight, electrochemically stable, affordable polymeric materials

Grand Challenge 7:

Educate the workforce of tomorrow to be well-versed in both experiment and simulation

If polymer scientists were educated and trained in an MGI-based environment (via physical and virtual colocation, curriculum development, scholarships, internships, or grants), including mentoring by multiple PIs – experimental and simulation - then we could

- Change the paradigm of materials discovery away from linear model to MGI model
- See tangible impact in 3-6 years
- Cross-pollinate scientific research via collaborative model

Breakout XYZ

"If materials scientists could _______, then new pathways of materials discovery would be possible."

If materials scientists could ________, then new pathways of materials discovery would be possible.
Have a framework for evaluating the accuracy of forcefields along with database of forcefields for a wide range of materials.

Use as many slides as needed

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"If materials scientists could ________, materials/product engineers would be able to ________.

If materials scientists could ________	Materials/product engineers would be able to _____
Understand and measure the sequence of monomers within a polymer	Comprehend, design, and tailor the properties for specific functions
Understand the connection between molecular characteristics and macroscopic behavior	Design materials for specific applications. Reduce the time required to match a material to the intended use.
Characterize the structure – for example branching	Could control the rheological properties and processibility of the polymer
Predict properties of multiblock polymers (beyond linear architecture)	Harness the more complex systems for 3D / functional materials

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If materials scientists could ________	Materials/product engineers would be able to _____
Understand how polymers behave and degrade under harsh environmental conditions (pressure, temp, stress, strain, oxidizing conditions, pH, current, adhesion, etc.)	Increase the application space for polymeric materials
Understand supramolecular assembly (where building blocks exceed atomic dimensions)	Obtain new classes of active / reversible materials
Synthesize polymers using many monomers (>> 3)	Increase the design space available to polymeric materials
Understood how charged polymers / ionomers behave	We could design materials that mimic the complexity of biosystems
Understood interfacial structure and behavior of thin films	Enable novel fabrication processes in a variety of application spaces (coatings, nanoelectronics, energy, etc)

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If materials scientists could ________	Materials/product engineers would be able to _____
Understand long time behavior of polymeric systems and material/ material interfaces	Predict and improve upon reliability for polymeric-based products (packaging, transportation, energy, etc.)
Understood polymer interfaces	Better coatings, integration, reliability
Characterize polymer materials in 3 dimensions in real time	Enhance the understanding of polymer properties and correlate to chemical structure / architecture
Develop minimal mesoscale models for prediction of structure, thermodynamics and rheology	Formulate tailor made materials for specific applications
Models that focus on mesoscale structure, morphology, properties, and rheology, without getting caught up in atomic level details	Predict the overall behavior of large classes of materials, identify important trends, discover new classes of structures and properties for innovative applications

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"Materials/product engineers need to be able to ________, which materials scientists could enable by _________."

Materials/product engineers need to be able to ______	Which materials scientists could enable by ______
Predict the behavior of multi-component polymer blends	Understanding the phase behavior of blended systems and the role that additives has on the resulting rheological properties
Design adhesives that can work in an aqueous environment	Understanding charged polymer behavior in solution as a function of environmental conditions
Fabricate circuits with < 10 nm dimensions	Providing materials that self-assemble or organize at this lengthscale (and below)
Predict how sequence and monomer composition influences polymer behavior and functionality, including when sustainably produced monomers are used for synthesis	Design, synthesize and produce polymers in a sustainable manner, and with target properties that are engineered from the bottom up.

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Materials/product engineers need to be able to ______	**Which materials scientists could enable by ______**
Design membranes that can withstand harsh environmental conditions (high pressure, variable water quality, etc)	Understanding the interfaces of the membranes; understand biofouling; understand charged interfaces and degradation mechanisms
Design lightweight, reliable batteries with high energy density	Understanding charge and electron transport; understanding thermal management; designing for these parameters; Designing / engineering multilayer stacks
Characterize materials in nanopatterned features or thin films	????
Manufacture a new class of monomers / materials from “bugs” (bio-produced)	New classes of materials that are readily scalable / sustainable