3. 학과내 연구실 소개

Dept. of Chemical and Biomolecular Engineering

이승익

지난회의 학과 및 교수소개에 이어 학과내의 주요 연구실의 연구주제와 현재 수행중인 프로젝트에 관하여 소개하고자 합니다. 이곳에서도 나노, 바이오, 연료전지가 가장 핵심적인 프로젝트로 활발한 연구가 진행중에 있습니다.

관심분야에 따라 현재 이곳에서 진행중인 연구정보를 알려줄 수 있는 기회가 되었으면 합니다.

◎ Boder Research Group

Eric T. Boder

Overview

The Boder Lab focuses on engineering proteins for various purposes, most notably for applications related to T cell immunology. The experimental approaches used are collectively called biomolecular engineering to emphasize the focus on molecular structure and properties. Numerous methods from molecular and cell biology are applied as non-traditional engineering tools with the goal of developing novel protein-based molecules for addressing current research, medical, and biomaterials needs.

Current Projects

- Development of a combinatorial library-based method for identification of CD4+ T cell activating peptide antigen sequences
- Engineering HLA-DR4 class II MHC for altered peptide binding specificity
- Development of a single-chain HLA-DR4 fragment
- Design and optimization of protein-based functional biomaterials
- Development of a novel recombinant mammalian expression system for engineering and analysis of cell surface receptors
- Optimization of sequence-specific biotinylation and development of a coupled expression/biotinylation methodology
- Surface expression of mammalian CD47 on yeast for assays of phagocytic response inhibition

http://www.seas.upenn.edu/~boder/

◎ Laboratory for Nanoscience and Molecular Engineering at Interfaces (NAMEI)

Russell J. Composto

Overview

Polymer Surfaces and Interfaces, Thin Films, Wetting, Dewetting, Polymer Blends, Diffusion, Ion Scattering and Cell Adhesion

Polymeric thin films are important to many current fields such as microelectronics, medical, and chemical industries. Presently, our research group is investigating phase separation and wetting in thin film polymer blends, patterning of polymer films, engineered surfaces for cell adhesion and growth, diffusion in filled systems (ionomers and polymer/silica blends), and dewetting of thin films with copolymer adhesion promoters. These projects use state of the art characterization tools including forward recoil spectrometry and neutron reflectivity for depth profiling, and atomic force microscopy and confocal microscopy for lateral profiling.

Current Research Topics

- Block Copolymer Adsorption at the Polymer/Substrate
- Functionalized surfaces for bone cell adhesion
- Investigation into the Local Environments of Acid Groups In Ionomers
- Surface Segregation and Nanostructure Formation in Ionomer Films
- Modulation of integrin-mediated adhesive properties of osteoblast cells using self-assembled monolayers (SAMs) with conformationally constrained RGD-mimetic peptides
- AFM Imaging of Supramolecular Cylindrical Structure of Ion Confined Self-Assembled Dendrites
- The controlled pore membrane by varying thickness, composition, and thermal history

http://www.lrsm.upenn.edu/~composto/intro.html

◎ Crocker lab

John C. Crocker

Overview

My research interests lie in biophysics, at the border between molecular and cellular biology with soft condensed matter physics. My group's expertise lies in figuring out how to make careful mechanical measurements on very small objects; to figure out what's going on in the micro-world. We use novel physical methods to probe interesting biological systems such as the cytoskeleton and complex macromolecules. Alternatively, we can use the power of biological systems to build interesting soft-matter experiments and engineer useful devices.

Cellular Biophysics

A major question we are presently pursuing is whether we can apply the principles of continuum mechanics to the cytoskeleton of living cells. Can we sensibly quantify the squishy-ness (rheology) of a cell using a frequency-dependent shear modulus? If so, how do we measure it? Does it bear any resemblance to the rheology of more conventional materials like entangled polymers or crosslinked gels? How does the presence of active elements (motors) affect a cell's rheology? How is the rheology adaptive vis-a-vis organelle motion or cell motility? One tool we use to answer these questions is particle tracking microscopy, where we use a computer to reconstruct the motion of small tracers imbedded in the cytoskeleton. We then can answer these questions by analysing the trajectories using high-powered statistical algorithms.

Molecular Biophysics

In another series of experiments we are trying to understand how a molecule called RecA works. RecA has the remarkable property that it can search through a large amount of double-stranded DNA and then selectively bind only to a prespecified sequence. To understand how it accomplishes this we are following the motion of single-molecular RecA complexes using particle tracking microscopy, while pulling on them with magnetic beads or optical tweezers.

Soft-Matter Engineering

Recently there has been a great deal of interest in 'self-assembly'. You put some objects together in a box and random motions and entropy assemble them into a structure you want. We are utilizing the specificity of DNA hybridization reactions (the tendency of the two halves of the double helix to bind each other) to 'program' self-assembly processes. Right now we are looking at methods of assembling bacteria-sized plastic beads (called 'colloids') into complex, but ordered, three-dimensional structures.

If you'd like more details as to how we can simultaneously track hundreds of microscopic objects to a few nanometers, we have a software page here (http://glinda.lrsm.upenn.edu/~weeks/idl/.)

◎ Biophysical Engineering Lab-discher lab

Dennis Discher

Overview

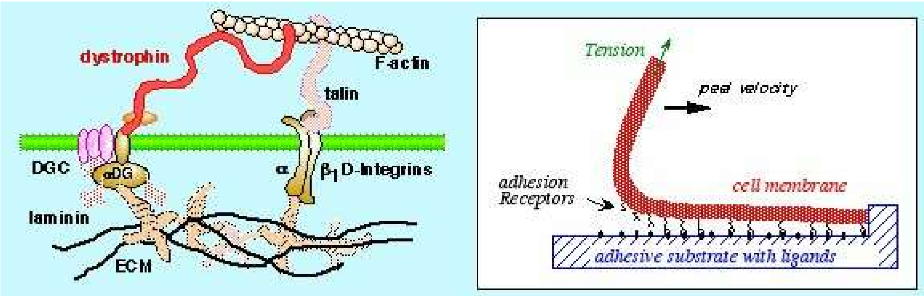
A unifying theme in the bulk of our studies is 'membranes'. Primary systems in focus include: 'marker of self' proteins on natural membranes, membrane skeletons and their component mechanics, membrane adhesion (muscle adhesion & Ig-CAM extensibility), copolymer-based mimics of biomembranes - "Polymersomes", physicochemical properties of the nucleus, liquid crystal elastomers.

- TOUGH POLYMERSOMES
- SINGLE MOLECULE EXTENSIBILITY

Single protein molecules are being stretched with molecular force probe techniques. Our primary focus is on cytoskeletal proteins such as spectrin and adhesion proteins such as VCAM-1. .Atomic Force Microscopy approaches are being employed in these single molecule studies and indicate that beta-spectrin can be forced to unfold. The first protein studied by these methods was an Ig-superfamily adhesion molecule known as Mel-CAM (P.N.A.S. Feb. 2001) a multi-domain protein -- a pre-requisite for such interrogation.

- MUSCLE CELL ADHESION MECHANICS

Growth and fusion (A-C) of muscle cells on mechanically-patterned substrates for the purpose of characterizing their adhesive mechanics (D-J) [in collaboration with the Sweeney Lab]. Journal of Cell ScienceApr. 1999. Present applications of the methods are to the study of dystrophic muscle cell which have defective cytoskeletal and adhesion components



- RED CELL MEMBRANE SPECTRIN-ACTIN CYTOSKELETAL MECHANICS: DISCRETE CYTOSKELETAL STRUCTURE IN DEFORMATION

Statistical mechanical simulation of a blood cell's spectrin membrane network held in a micropipette (Biophysical Journal75: 1584-1597 (1998)). Current simulations are focused on the role of actin protofilaments.

http://www.seas.upenn.edu/~discher/

◎ RJG research group

Raymond J. Gorte

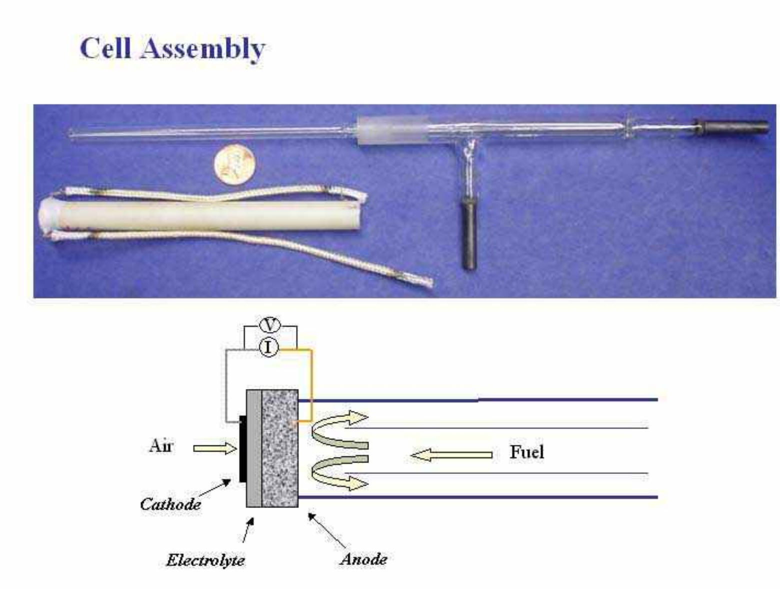
Current Focus of Research:

Automotive Emissions Control Catalysis

Current automotive catalysts are a complex mixture of precious metals and various oxides. Meeting present standards for NO, CO, and hydrocarbons requires that the interactions between the various components be carefully engineered. This is especially true for the oxygen-storage component, a critical part of the catalyst which controls the oxygen stoichiometry by means of a reducible oxide, usually ceria. We have shown that the reducibility of ceria, and its interaction with the precious-metal components, depends strongly on the structure of the ceria and the presence of various dopants. We use a wide variety of techniques to study this affect, range from measurements of reaction kinetics, electron microscopy, isotope-labelling studies, and low-angle, x-ray scattering. The goal is to develop a better understanding of those factors which influence the catalytic properties.

Anodes for Solid-Oxide Fuel Cells

Solid-Oxide Fuel Cells (SOFC) offer an attractive alternative to gas turbines for generating electricity. In SOFCs, oxygen anions are transported through an oxide membrane and react with the fuel at the anode. A major problem is that typical anode materials are only active enough to work with hydrogen, so that practical fuels, like methane, must first be steam reformed to hydrogen. This imposes severe limitations on the operating conditions. We are using concepts developed from our program in automotive catalysis to synthesize anodes which are active for the direct oxidation of hydrocarbon fuels. This work involves building model SOFCs and performing spectroscopic studies of the anodes.



Zeolite Acidity

Zeolites are used as acid catalysts for a wide variety of reactions in the chemical and petroleum industry. While there is potential for using them for even more reactions of commercial interest, acidity in solids is not defined well enough to adequately control the conditions under which reactions occur. We use a number of techniques, including TPD mass spectroscopy, NMR, microcalorimetry, and infrared spectroscopy to characterize adsorbates and potential reaction intermediates so as to understand the fundamental processes which take place at the acid sites. Some of the techniques we have developed are already being applied by several major catalyst companies for the characterization of commercial catalysts.

http://www.seas.upenn.edu/cbe/gorte.html

◎ Hammer laboratory

Daniel A. Hammer

Overview

The Hammer laboratory uses physical principles to understand and manipulate the behavior of biological systems. Penn is an excellent location for such research, with strength in the physical sciences, engineering and a first-class medical school -- all located on a single campus.

Cell adhesion: We are interested in how cell adhesion is controlled by the physical and chemical properties of cell surface molecules. Using biological cells and molecules, well-defined adhesion assays, and computer simulations, we are developing a comprehensive picture of how cell adhesion molecules work. We have reconstituted adhesion molecules from white cells onto polymeric spheres, retaining full molecular activity.

Virus-cell interactions: Our lab studies the fundamental factors that control viral infection, especially membrane fusion, where the outer lipid bilayer of the virus fuses with a membrane of the host cells. This fusion is mediated by proteins on the viral surface. Our long-term goal is to reconstitute the fusion activity of viral molecules into larger structure, using artificial molecular fusion machines.

Polymersomes: With collaborators, we have been able to make vesicles from diblock copolymers. These vesicles, called "polymersomes" are tougher and less permeable than phospholipid vesicles, and thus offer advantages for drug delivery and encapsulation. We are working on making polymersomes from new polymers and assessing biological applications of the resulting structures.

http://www.seas.upenn.edu/be/daniel_hammer_details.html

◎ Seider research group

Warren D. Seider

Multiphase Equilibria and Azeotropic Distillations

Advances in the calculation of multiphase equilibria are crucial for the successful simulation of heterogeneous azeotropic distillation towers, especially in the presence of salt-water solutions, where electrolytic reactions can lead to salting-out on the trays. Hence, a focus of our work is on the implementation of stability analysis, using the tangent-plane-distance function, to better locate trial phases for the minimization of the Gibbs free energy. In the design and control of these towers, the interfaces between trays having two- and one-liquid phases(s) are very sensitive to the reflux rate. We seek improved strategies for studying the dynamics of these towers and the existence of multiple steady states under normal operating conditions.

Design and Operation at Unstable Steady States

Many processes have been overdesigned because engineers are reluctant to design near or within regimes of complex operations, where they are often economically optimal. This is prevalent in processes with exothermic and autocatalytic reactions and where phases appear and disappear, especially in the critical region. We are developing designs that operate more economically closer to these nonlinear regimes, which are characterized by multiple steady states, periodic and even chaotic operation, often exhibiting inverse response. Improved control strategies are being developed to permit reliable operation near these regimes.

Nonlinear Model-based Controller Design for Non-minimum-phase Processes

To achieve more effective process designs, nonlinear model-based controllers are being developed for processes with a non-minimum-phase, delay-free part. The controllers are derived by exploiting the connections between model-predictive and input-output, linearization controllers, and are designed to satisfy input constraints. The performance of the control laws is illustrated using numerical simulation and real-time experiments. Special challenges arise when the process exhibits both non-minimum-phase and unstable steady states. In one approach, we seek to alter the design to modify the process dynamics. Using bifurcation analysis, optimization algorithms, and the addition of sensors and actuators, proposed design changes are explored more effectively.

Controller Verification Under Uncertainty

To deal with uncertainties in process design and control, we are developing strategies for the verification of the stability and performance of controllers. Emphasis is placed on situations when both parametric and non-parametric uncertainties exist in the process model. In one approach, a qualitative reasoning technique, using symbolic manipulation, is being created to construct bounding equations. We are also developing a non-parametric Monte Carlo technique. These techniques are being applied for the automatic verification of control actions to prevent the process from straying into hazardous regimes in the face of large disturbances and faults.

Plant Design for Ease of Transition

Through the design of multi-product plants, using the same equipment, capital expenditures are often reduced. In continuous processing, transitions from one product to another are carried out often without shutting down the process; for example, in gas-phase, co-polymerization plants. We seek design strategies that simplify the transitions between many different product grades. To accomplish this, design optimizations account for transition costs, in addition to the costs of steady-state operation. Strategies involving the optimal sequencing of transitions are being developed; for example, to select among scenarios involving the manufacture of products A, C, and B, in sequence, rather than the manufacture of products A, B, and C, in sequence. Objectives include the reduction of transition times and off-specification product.

Semicontinuous Distillation

Traditionally, distillation processes are designed to operate either in batch or continuous modes. In the former, process efficiency is sacrificed for separation flexibility, whereas in the latter, operational efficiency is gained at the cost of process flexibility. As a departure, we have been developing semicontinuous approaches that share the advantages of both modes. Our work concentrates on the development of semicontinuous campaigns for the separation of multicomponent mixtures, including azeotropes and simple distillation boundaries.

Czochralski Crystallization

Recent work involves the design of distributed parameter systems with momentum, heat, and mass transfer and complex boundary conditions. For the real-time control of Czochralski crystallizers, we have been creating a model-predictive controller that utilizes a reduced-order model to capture the convective patterns in the melt and its boundary layers.

Fluid Flows at High Convection Levels

In industrial-scale Czochralski crystallizers, convection in the melt dominates over diffusion processes, leading to finite-element models that require the solution of large systems of linear equations, whose coefficient matrices are non-diagonally dominant, non-symmetric, and highly indefinite. These matrices are difficult to invert, even using iterative methods, because of excessive accumulation of round-off errors and the dependence of convergence properties on their eigenvalues. We are developing iterative geometric methods, based upon orthogonal projections, that do not suffer from the disadvantages incurred in the use of common iterative methods.

http://www.seas.upenn.edu/%7Eseider/seider.html

◎ Vohs research lab

John M. Vohs

Research Programs in Surface and Interfacial Science

Chemical processes which occur on surfaces and at interfaces are important in a variety of technologies ranging from chemical processing and manufacturing to electronic materials. The primary focus of the Vohs research group is to provide molecular level descriptions of a variety of chemical phenomena which occur on surfaces. Specific research projects currently encompass several areas including the mechanisms of surface-catalyzed reactions, thin film growth in electronic materials device fabrication, and the chemistry of polymer-metal interactions. The unifying theme of of these projects is the elucidation of the relationships between surface structure, chemical reactivity, and electronic properties. The experimental approach relies on the use of well-defined model systems that facilitate detailed surface structural analysis and the study the reactivity of these surfaces toward probe molecules. Surface reactions and adsorbed species are studied using a battery of ultra-high-vacuum surface analysis techniques including, temperature programmed desorption (TPD), X-ray photoelectron spectroscopy (XPS) and high resolution electron energy loss spectroscopy (HREELS).

Surface Science Studies of Model Supported Vanadia Catalysts (funded by NSF)

V_2O_5 supported on TiO_2 and other oxides is known to exhibit unusually high activity for a variety of selective oxidation reactions including the oxidation of o-xylene to phthalic anhydride, the oxidation of alcohols to aldehydes and ketones, and the ammoxidation of aromatic hydrocarbons. Characterization studies have shown that the active phase in V_2O_5/TiO_2 catalysts is composed of a two-dimensional V_2O_5 overlayer composed of either isolated vanadyls or polymeric vanadates. The isolated vanadyl has three oxygens bridging between the support and the vanadium ion and a single terminal V=O bond. It has been suggested that the terminal V=O bond is the active site for selective oxidation reactions and that interactions with the support alter the strength of this bond and the reactivity of the surface vanadia complex. Recent experimental results are inconsistent with this description, however. For example, it has been shown that the activity for methanol oxidation does not correlate with the V=O bond strength. Based on this result, it has been proposed that the bridging support-O-V bonds are the active sites for reaction, rather than the terminal V=O bonds and that the dependence of the reactivity on the identity of the support is due to variations in the reduction characteristics of the V-O-support bonds. Unfortunately, the strength of the vanadia-support bonds has yet to be directly measured. Thus, a correlation between reactivity and the strength of these bonds is still not firmly established.

In this research project, model catalysts composed of submonolayer, monolayer, and multilayer films of V_2O_5 supported on the surfaces of metal oxide single crystals are being studied with the goals of determining the active site for selective oxidation reactions on supported monolayer V_2O_5 catalysts and elucidating the nature of the synergistic effect between the vanadia layer and the support. In these studies, the reactivity of the model catalysts is being probed using temperature-programmed desorption (TPD), while the structure of the supported vanadia phases are being characterized using a combination of low energy electron diffraction (LEED), Rutherford backscattering spectroscopy (RBS), and high-resolution electron energy loss spectroscopy (HREELS). The HREELS experiments are focusing on characterizing differences in the V-O-support bonds for the various substrates.

Fundamental Studies of Automotive Emissions Control Catalysts

This project involves collaborations with Professor Gorte and Professor Egami

(Funded by DOE)

Automotive emissions control catalysts are used to oxidize CO and hydrocarbons in engine exhaust as well as reduce the level of smog producing NOx species. The primary active components in these catalysts are Pt group metals (i.e. Pt, Pd, and Rh) supported on a-alumina. A variety of oxide promoters, the most important of which are CeO2 and ZrO2, are also used. Although it is well established that interactions between the metals and the oxide promoters are critical in maintaining both catalyst activity and durability, a detailed understanding of these interactions is still lacking. It is clear, however, that a fundamental understanding of these interactions and developing ways to enhance them is key to the development of the next generation of automotive catalysts which are able to meet or exceed recently enacted federal emissions control regulations.

In this research program we are using a variety of surface sensitive spectroscopic probes including, X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES), and high resolution electron energy loss spectroscopy (HREELS) to characterize interactions at Pt-group metal-ceria and Pt-group metal-zirconia interfaces and how these interactions influence catalyst reactivity. The kinetics of surface reactions are being monitored using temperature programmed desorption (TPD). To date we have demonstrated that under fuel rich operating conditions ceria is able to undergo reduction and release oxygen which can then react with CO adsorbed on the supported metals. This reaction pathway appears to be important in maintaining catalyst oxidation activity under rich operating conditions. The mechanism by which oxygen is transferred from the ceria to the metals is still not well understood, however. We have also shown that the extent of reduction of the ceria surface has a profound effect on reactivity. For example, enhanced dissociation of CO has been observed on Rh supported on partially reduced CeO2 compared to Rh supported on fully oxidized CeO2. It is interesting that this reaction pathway is not observed for Pd and Pt supported on reduced ceria. These results demonstrate that the interaction of the Pt-group metals with ceria and the resulting effect on reactivity is highly structure sensitive and depends on both the identity of the metal and the structure of the ceria surface.

Conducting Polymer-Metal Interfaces

(Funded by NSF through the MRSEC program)

Due to their unique electronic properties and ease of processing, electrically conducting polymers such as polyaniline, polyacetylene, and polythiophene have potential in applications ranging from electroluminescent layers in flat panel displays to chemical sensors. In most if not all of these applications the conducting polymer is present as a thin film. As a result, interactions between the polymer layer and a solid substrate can influence both the mechanical and electronic properties of the device. The goal of this research project is to elucidate the nature of the chemical bonding at conducting polymer-metal and conducting polymer-metal oxide interfaces and determine how these bonding interactions influence both the structure of the polymer layer and its electronic properties.

To date the primary focus of this research program has been on characterizing the structure of vapor-deposited films of polyaniline on Cu, Ag, and Au substrates with emphasis on understanding chemical interactions at the interface. The primary experimental technique used in these studies has been high-resolution electron energy loss spectroscopy (HREELS). In this project we are using a new design of HREEL spectrometer that has extremely high-energy resolution thereby allowing us to characterize the vibrational spectrum of thin polymer films in unprecedented detail. We have recently shown that on Cu substrates, polyaniline is covalently bonded to the surface through Cu-N bonds, while on Au substrates, Van der Waals interactions predominate. These differences in the mode of bonding at the interface result in the polyaniline thin films having different structures on the two substrates. The polyaniline films are more highly ordered on Au relative to Cu. This in turn has a dramatic effect on the conductivity of the polyaniline films upon doping with HCl. The highly ordered films on Au exhibit an unusually high conductivity.

In addition to studying the bonding interactions at the polyaniline-metal interfaces we have also characterized the chemistry of the vapor deposition of polyaniline thin films. We have demonstrated that the growth process consists of the adsorption of relatively short oligomers (3-5 aniline units in length) which then react on the surface to form higher molecular weight material. The degree of branching along individual polymer chains was also found to increase with increasing film thickness.

Surface Chemistry of MOCVD Processes
(Funded by NSF)

Metalorganic chemical vapor deposition (MOCVD) is an important technique for the growth of thin films of electronic materials such as ZnSe and GaAs. In this project we are studying the surface chemistry of metalorganic precursors on semiconductor substrates. The primary focus of this project is to elucidate the surface reaction mechanisms of the precursor molecules and to determine how the structure of the substrate influences reaction chemistry and film nucleation. Specific systems that are currently being studied include the growth of ZnSe, GaN, and GaAs using metalalkyl precursors

http://www.seas.upenn.edu/~vohs/JMV_research.html