Notes on Scientific Session: 'Nanotechnology as it Interfaces with Material Science and Imaging'

By Mary Walker (UMKC School of Dentistry, Oral Biology and Restorative Dentistry)

Dr. Shubhra Gangopadhyay from the Electrical and Computer Engineering Department at the University of Missouri-Columbia spoke about "Nanoscale Self-assembly and its Applications in Material Science." She described her research group efforts that are focused on the integration of top down semiconductor and MEMS (microelectromechanical system) processes with bottom up self assembly based chemical synthesis processes. They have several ongoing research projects funded by NSF, DoD and NIH in the areas of biosensors, nanoengineered energetic materials, bulk and thin films with ordered and random pores and high dielectric constant materials. She and her collaborators are working on microchip-based sensing systems such as the microfabrication of an optical system for fluorescence detection that could be used for HIV virus detection. Other projects include an electrochemical sensing device to detect small amounts of chemical release such as catecholamine and micro-fluidic assay to quickly analyze microscopic samples of DNA for field applications. The research group is also currently working on a new approach for self-assembling fuel and oxidizer nanocomposites on chip and utilizing semiconductor chip processing for many applications. Professor Gangopadhyay's collaborators include Drs. Sheila Grant, Kevin Gillis, Steve Kleiboekker, Lela Riley, Rajsh Shende, and Keshab Gangopadhyay.

"Structure, Property and Functional Imaging from Nano- to Micro-Scales" was presented by Dr. Yong Wang, Oral Biology Department at the University of Missouri-Kansas City School of Dentistry. He explained the need for structure/property/function characterization of the material/tissue interface as new materials are developed for tooth restorations to major reconstruction of facial hard and soft tissues. He described some of the technology available at the Center for Research on Interfacial Structure and Properties (UMKC-CRISP) such as confocal microspectroscopy, FTIR chemical imaging, micro-mechanical measurements with scanning acoustic microscopy and atomic force microscopy. This instrumentation is being used to determine the interfacial structure/property/function relationships of synthetic materials with natural tissues, e.g., bone, dentin, enamel and collagen. The combination of imaging and microscopy provides a means for relating structure, chemical and mechanical properties from micro- to nano-scales. The data provide an integrated analysis which is critical to their research efforts to define factors and/or mechanisms that lead to premature breakdown of materials during clinical function.

Dr. Anil Misra, Department of Civil and Mechanical Engineering at University of Missouri-Kansas City, discussed "Nano and Micro-Scale Mathematical Models." His presentation included a description of mathematical models he has developed to predict stress and strain at the dentin/adhesive interface in tooth colored dental composite restorations during clinical function. He also discussed modeling he and his research colleagues have done related to nanometer thin intergranualar glass films (IFGs) that form in polycrystalline ceramics during sintering and the IGF structure and property changes related to doping with rare earth elements. Theroretical experiments using *ab initio* calculations of the mechanical properties of both undoped and a Yittria-doped IGF model have been performed. Their results indicate interesting differences between the stress-strain response of undoped and Y-doped models. To relate the *ab initio* calculations to the continuum scales, they analyzed the atomic-scale deformation field under uniaxial loading. The deformation pattern obtained through the *ab initio* calculations indicates that it is possible to construct discrete grain-scale models that may be used to bridge the calculations to the continuum scale.

Dr. Kartik Ghosh from the Department of Physics, Astronomy, and Material Science at Missouri State University described research conducted at MSU in the area of magnetic nanostructures for spintronic devices. The facilities at MSU include thermal evaporation, RF sputtering, a pulsed laser deposition system, molecular beam epitaxy equipment, spin coaters, a mask aligner, scanning probe microscope equipped for magnetic and electrical force microscopy, scanning electron miscropscope, a micro-Raman spectrometer, and photoluminescence apparatus.

Dr. Jee-Ching Wang, University of Missouri-Rolla Chemical and Biological Engineering Department, presented "Applications of Atomistic Computer Simulations in Nanoscience and Bioseparation." He explained how molecular simulations represent a powerful, new research tool for both engineers and scientists. These computer experiments in principle can be used to calculate physical and chemical properties of model systems under controlled conditions to help identify molecular origins of important phenomena and to characterize the relative importance of different mechanisms and parameters. They have used molecular dynamics (MD) simulation technique to study the transport and adsorption of a positively charged biomolecule (desmopressin) onto a negatively charged solid surface. Their results indicate that the transport and adsorption mechanisms are dominated by Coulombic interactions, i.e. electrophoretic migration. During adsorption, desmopressin is induced to change its structure and size, which can have significant consequences in bioactivity and bioseparation. As the molecule approaches the surface, its perpendicular mobility increases but its lateral mobility decreases and becomes practically zero in its adsorbed state. These differences and changes in the values of transport coefficients have important implications with respect to the replenishment of the biomolecules in the inner parts of a channel (pore) and the overall rate of adsorption. Specifically, the realization of effective transport and overall adsorption rate require the pore radius of porous adsorbent media to exceed certain critical value. A novel method was presented to estimate this lower bound of the pore radius, which is based on the information from their simulation studies about the sizes of desmopressin molecules in the adsorbed layer and in the liquid layers above as well as the number and size of the hydration layers around desmopressin molecules.

Dr. Steven Buckner, Department of Chemistry, St Louis University, presented “Long Period Gratings and Luminescence Nanoparticles: Nanomaterial-Based Sensors.” He explained how simple nanostructured materials can provide reliable and selective platforms for a variety of chemical sensing applications. He also described two examples of such systems. In the first example, long-period-grating (LPG) fiber optic sensors are coated with a nanoscale thin film of carboxymethylcellulose. This film selectively binds Cu^{2+}. Upon binding, the polymer collapses producing a density increase. This density increase induces a modulation in the spectral loss element in an LPG fiber. They have monitored the time-dependent response of the wavelength modulation and developed a kinetic scheme to model the behavior of this system. Using this approach an analytical scheme is developed providing sub-ppm limits of detection for Cu^{2+}. In the second example, he and his collaborators use the luminescence quenching behavior of PbS nanoparticles as a method for detection of water. There are a variety of methods for water detection and quantification in materials, Karl-Fisher titrations being the most common. Optical detection schemes for water in condensed materials are notoriously non-selective. Luminescence quenching of nanoparticles in polymer films was presented as a method for selective detection and quantification of water.
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Dr. Sanju Gupta from the Department of Physics, Astronomy, and Materials Science at Missouri State University presented “Nanostructured Carbon Materials: Carbon Nanotubes and Conducting Polymer Polypyrrole.” Carbon nanotubes – elongated members of fullerenes – serve as a model example of nanoscale science and technology. Severe environmental tolerability is the prime factor in the development of novel space materials accompanied by lightweight, reusability, and multifunctional capabilities. In the first part of the talk, an example of carbon nanotubes for space applications was presented. Because it is critical to demonstrate that these materials are physically stable and structurally unaltered when subjected to irradiation, microwave CVD deposited carbon nanotube films were subjected to low and medium energy electron-beam irradiation to study its influence on structure and the corresponding physical properties and establish *Be-structure* correlations. Microstructural and physical properties characterizations were made prior to and post-irradiation include scanning electron microscopy (*SEM*), atomic force microscopy (*AFM*), Raman spectroscopy (*RS*), X-ray diffraction (*XRD*), field emission (*FE*), and high-resolution transmission electron microscopy (*HRTEM*). In the second part of the talk, controlled synthesis of conducting polymer polypyrrole (PPy) nanostructures was discussed. Polypyrrole in the family of π-conjugated polymers is a potential candidate for building microscopic actuators, electrochromic devices, and drug delivery systems. Dr. Gupta and her colleagues have used electrochemical technique to polymerize pyrrole onto stainless steel substrates from electrolytes (organic solvent, supporting electrolyte, and monomer) in a single compartment three-electrode cell. Experimental results show that surfactant-mediated growth under controlled electrochemical biasing led to synthesis of micro/nanostructures. sxg535f@missouristate.edu