NIST/Industry Polymer Surface/Interface Consortium Meeting

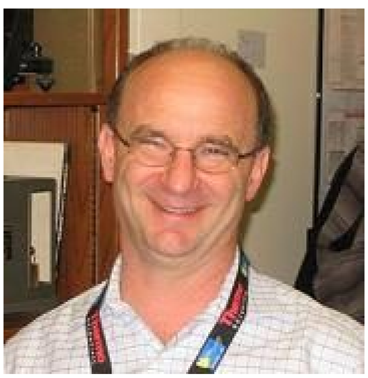
September 17, 2019, Tuesday, *Conference Room: Lecture Room A/Bldg 101*
Industrial Practice and Scientific Exchange (Invited presentations)

8:40- 9:00	Social networking
9:00- 9:10a	**Welcome, Jason Averill, Division Chief** ***Materials and Structural Systems Division*, *EL***
9:10- 9:40a	**Polymer Physics of 3D Printing** Dr. Kalman Migler, *Materials Science and Engineering Division*, *MML*
9:40 – 10:10a	**Additive Manufacturing with Cementitious Materials** Dr. Scott Jones, *Materials and Structural Systems Division, EL*
10:10 – 10:30a	Break
10:30 – 11:00a	**MGI and AI** Dr. James Warren, Director, *Materials Genome Program*, *MML*
11:00– 11:30a	**Databases for polymer informatics** Dr. Debra J. Audus, *Materials Science Engineering Division*, *MML*
11:30a– 12:00p	**Surface and Trace Chemical Analysis using Time-of-Flight Secondary Ion Mass Spectrometry** Dr. Shin Muramoto, *Materials Measurement Science Division*, *MML*
12:10- 1:10p	Lunch at NIST Cafeteria
1:20 – 2:20p	**Tour: EL AM Research Center (AMRC) in 304/124** Dr. Thien Phan, *Intelligent Systems Division, EL*
2:30- 3:00p	**Demo: Data Augmented 360-degree Video** Dr. Matthew Hoehler, *Fire Science Division, EL*
3:00 – 3:20p	Break
3:20 – 3:40p	**Testing Polymeric coatings** Dr. Pierre Morel, *Rtec Instruments*
3:40- 4:10p	**Investigating home and automobile exterior performance after weathering** Dr. Ronald Lankone, *Materials and Structural Systems Division*, *EL*

Polymer Physics of 3D Printing

Dr. Kalman Migler, Materials Science and Engineering Division, MML/NIST

Material extrusion (ME) is a layer-by-layer additive manufacturing process that is now used in personal and commercial production where prototyping and customization are required. However, parts produced from ME frequently exhibit poor mechanical performance relative to those from traditional means; moreover, fundamental knowledge of the factors leading to development of inter-layer strength in this highly non-isothermal process is limited. Here, we seek to understand the development of inter-layer weld strength from the perspective of polymer interdiffusion under conditions of rapidly changing mobility. Our framework centers around three interrelated components: in-situ thermal measurements (via infrared imaging), temperature dependent molecular processes (via rheology), and mechanical testing (via mode III fracture). We develop the concept of an equivalent isothermal weld time and test its relationship to fracture energy. The results of these analysis provide a basis for optimizing inter-layer strength, the limitations of the ME process, and guide development of new materials.



Dr. Kalman Migler leads the Polymers-based Additive Manufacturing and Rheology Project for the National Institute of Standards and Technology, where he has worked for 25 years. His primary interest is in the measurement of non-equilibrium phenomena that occur during polymer processing. Throughout his career he has developed technologies to measure polymer blend extrusion, polymer processing instabilities, fluoropolymer additives, polymer slippage and carbon nanotube composites. Before joining NIST, he was a postdoctoral research fellow at Exxon's Corporate Research Laboratory and at the Collège de France. He earned his Ph.D. in Physics from Brandeis University. He is a Fellow of the American Physical Society, the Society of Rheology and of the Washington Academy of Sciences. http://www.nist.gov/mml/msed/polymers/kalman-migler.cfm

Additive Manufacturing with Cementitious Materials

Dr. Scott Jones, *Materials and Structural Systems Division, EL*

Abstract: Additive Manufacturing with cement-cement based materials is an emerging technology that has the potential to revolutionize concrete construction. The placement process is quite complex, requiring sufficient flow properties as the material leaves the nozzle, and sufficient stiffening properties before the subsequent layer is placed. Precise control of material proportions and in-line monitoring of the time-dependent rheology are required to ensure the successful adoption of AM in the concrete. Connecting microstructure evolution of hydrating cement systems to macroscopic properties is critical to the success of this technology.

Bio:
Dr. Scott Z. Jones is a mechanical engineer in the Inorganic Materials Group of the Materials and Structural Systems Division (MSSD) of the Engineering Laboratory (EL) at the National Institute of Standards and Technology (NIST).
Dr. Jones received his Bachelor of Science degree (2009) and a Ph.D. (2016) from University of Maryland, Baltimore County. His dissertation focused on predicting the service life of reinforced concrete structures repaired with polymeric crack-filling materials.
Dr. Jones arrived at NIST through the NIST-America Recovery and Reinvestment Act (ARRA) fellowship program in 2011. He was a Pathways student intern at NIST from 2014 to 2016 where his research focused on modeling the transport of chlorine into cracked concrete structures. Dr. Jones' current research focuses on additive manufacturing techniques for concrete construction applications. He is the project leader of the Additive Manufacturing with Cement-based project, chair of ACI 564 3-D Printing with Cementitious Materials, and director of the Metrology of Additive Construction by Extrusion (MACE) consortium.

MGI and AI

Dr. James Warren, Director, *Materials Genome Program, MML*

US Materials Genome Initiative, a multi-agency initiative designed to create a new era of policy, resources, and infrastructure that support U.S. institutions in the effort to discover, manufacture, and deploy advanced materials twice as fast, at a fraction of the cost. More information about the MGI can be found at the MGI home page.

Bio:
Dr. Warren has been employed at NIST since 1992, in the Metallurgy Division and its successor the Materials Science and Engineering Division, within the Material Measurement Laboratory. He is also one of the co-founders, and the current Director, of the NIST Center for Theoretical and Computational Materials Science. Since 2010, Dr Jim Warren is the Director of Materials Genome Program, working with a government-wide team to build out the materials innovation infrastructure needed to realize the goals of the initiative. NIST, in particular, has an outsize role to play in achieving those goals.

Dr. Warren's research is broadly concerned with developing both models of materials phenomena, and the tools to enable the solution of these models. Specific foci include solidification, pattern formation, grain structures, wetting, diffusion, and spreading in metals.

Databases for polymer informatics

Debra J. Audus, Materials Science and Engineering Division, MML/NIST

Abstract:

Significant barriers to polymer informatics still remain---a lack of large, accessible datasets, a lack of infrastructure, etc. To reduce these barriers, we developed pipelines to harness the vast quantities of valuable experimental polymer data trapped in the literature. In our first effort, we developed the largest Flory-Huggins chi parameter database using crowdsourcing and found that the burden to review papers could be lessened by training a classifier to identify promising articles. To further reduce human input, we turned to natural language processing software coupled with specially designed software modules to extract grass transition temperatures with minimal human input; ultimately, we extracted over 250 glass transition temperatures. All of the resulting data is freely available at the Polymer Property Predictor and Database website (http://pppdb.uchicago.edu). During this process, we found that identification of the polymer names within the literature was a key problem as polymers are referred to by common names, sample names, labels, etc. and subsequently explored named entity recognition to tackle this problem. Finally, I will highlight some of the other efforts at NIST that aim to reduce the barriers to polymer informatics including the development of a more efficient code for computing hydrodynamics properties of polymers called ZENO and a pilot project under the NIST center for excellence, CHiMaD, in collaboration with ACS and RSC to release virtual issues in multiple journals where the polymer data is published along with the journal articles.

Bio:

Debra J. Audus is a staff scientist in the Materials Science and Engineering Division at the National Institute of Standards in Technology (NIST). Following her Ph.D. at University of California, Santa Barbara focusing on the nanostructured polyelectrolyte gels, she joined NIST as an NRC postdoctoral fellow before transitioning to staff in 2015. Her research interests include polyelectrolyte micelles, polymer crystallization, hydrodynamic properties of dilute solutions, polymeric databases, and machine learning.

Surface and Trace Chemical Analysis using Time-of-Flight Secondary Ion Mass Spectrometry

Shin Muramoto, Materials Measurement Science Division, MML/NIST

The Surface and Trace Chemical Analysis group at the National Institute of Standards and Technology (NIST) is involved in a research program for the forensic analysis of narcotics, particles, paint, and nuclear materials. In parallel to this effort, the group is involved with the Department of Homeland Security (DHS) for the improvement and standardization of deployed trace explosives and narcotics detection systems. The program goals are very similar, with the ultimate goal of developing new measurement tools for the preparation of well characterized and quantitative test materials to evaluate the performance of current and next generation detection systems. The fabrication of realistic test materials is rather complex and require understanding of the nature of the analyte, such as explosive particles, in terms of their microchemistry, size distributions, adhesive and aerodynamic properties, and the extent to which these properties govern our ability to effectively sample and detect these particles. For example, analysis of particles in conventional explosives have shown that trace residues are not typically found in isolation but are rather associated with high levels of environmental background such as soils and fingerprint residue, which may negatively influence the performance of trace detectors. To this extent, the use of advanced microanalytical and surface analysis techniques is a critical component of this program. One such example is the time-of-flight secondary ion mass spectrometer (ToF-SIMS) that can provide chemical information from solid surfaces with monolayer sensitivity and sub-micrometer spatial resolution. It is capable of effectively detecting particles inside complex matrices, such as fingerprints, and can detect monolayer of molecules on the surface of micrometer particles. Combined with the argon gas cluster source, ToF-SIMS has provided 3D chemical images of drug particles in thin films as well as sub-surface layer structures in automotive paint layers. In addition, our interest in the characterization of fingerprint residue as a background matrix has led to forensically relevant findings such as the transfer efficiency of particles from hands to surfaces, depth of particles embedded in fingerprint, and the dynamic nature of the latent fingerprint that could be exploited to determine its age. The long-term goal is to have a flexible set of materials, methods, and know-how for the detection of not only existing explosives and narcotics, but a wide range of emerging threats and non-threat materials, to which ToF-SIMS has and will provide critical chemical information and solutions.

Bio:

Shin Muramoto is a research scientist at the National Institute of Standards and Technology (NIST). He graduated from the University of Washington with B.S. and Ph.D. degrees in Chemical Engineering, focusing on the functionalization and characterization of surfaces for biomedical devices. His current research directions involve characterization of thin films, particles, and trace residues using surface analytical techniques for homeland security and forensic applications.

Data Augmented 360-degree Video Demo

Dr. Matthew Hoehler, Fire Science Division, EL

NIST's Fire Research staff designed, fabricated, and tested a transparent, water-cooled enclosure to house cameras to record video from inside a fully-developed fire. This tool captures visual fire data in virtual reality to augment fire data collection and visualization.

Bio:

Dr. Matthew Hoehler is a Research Structural Engineer in the Engineering Laboratory at the National Institute of Standards and Technology (NIST). He provides program and technical support to the National Earthquake Hazards Reduction Program and the National Fire Research Laboratory to further NIST´s mission to ensure a resilient national infrastructure. Dr. Hoehler has over fifteen years of experience in experimental testing and analysis of the performance of materials, components, and structures associated with structural collapse, natural disasters, or human-initiated events.

Prior to joining NIST in 2014, Dr. Hoehler worked in the management and execution of applied research for private and public entities in the United States and Europe. He is the author of numerous technical publications in areas including full-scale testing of structural and nonstructural building systems, fastening technology, modeling and behavior of reinforced concrete structures, and measurement science. He has been an associate member of American Concrete Institute (ACI) Committee 355 "Anchorage to Concrete", International Federation for Structural Concrete (fib) Special Activity Group "Fastenings to Concrete and Masonry" and a contributor to the European Committee for Standardization (CEN) Working Group for the Technical Specification "Design of Fastenings for Use in Concrete."

Testing Polymeric coatings

Rtec Instruments develops and manufactures advanced mechanical and surface testing and measurement solutions for research and industrial applications. We specialize in combining techniques to provide unique perspective in material testing. Our testers include tribometer (tribology testing equipment), scratch tester (coating scratch adhesion tester), optical profilometer, fretting tester (fretting wear tester), hot hardness tester.

The presentation will review the applications of these instruments for testing polymeric coatings using tribology, scratch testing combined with the 3D inline imaging.

Bio:

Pierre Morel is a R&D engineer passionate and expert in indentation, scratch and tribology testing. Using 20 years of experience in material testing instruments he designs and supports Rtec Instruments for surface characterization. In addition to a MBA from George Washington University, he holds a master's degree in mechanical engineering from ENISE, and a second Master's degree in Materials Science from the University of Tennesse Knoxville.

Investigating home and automobile exterior performance after weathering

Ron Lankone, Materials and Structural Systems Division, EL/NIST

Polymeric exterior materials are the outer most barrier between occupants of a home or automobile and the surrounding environment. For homes, vinyl siding (polyvinyl chloride sheets) has grown over the last several decades to be one of the most popular siding materials in the United States due to its low cost, ease of installation, and aesthetic versatility. For automobiles, more recently, nanoform pigmented coatings have received increasing interest for their desirable color and gloss properties. Both exteriors will inevitability wear due to ultraviolet driven photodegradation, resulting fading, cracking, chalking, and/or an overall loss of performance. The NIST SPHERE, natural weathering, and an aggressive artificial weathering procedure, *The Kalahari Protocol*, were utilized to investigate the degradation behavior of home siding and an automobile coating with the explicit goal of determining the relationship between molecular level degradation and loss of exterior performance. Results demonstrate that for both exterior materials, changes in appearance after UV exposure correlate well to deterioration of the material, as measured by infrared spectroscopy. Furthermore, findings also indicate that changes in appearance, molecular degradation, and loss of mechanical performance all systematically increase with increasing UV exposure. The observation of this relationship permits the use of appearance measurements to predict the extent of material degradation; this is particularly useful in assessing the aging of vinyl siding and will be discussed. Lastly, discussion will cover preliminary fire testing studies of vinyl siding and focus on comparisons of fire performance as measured by different fire testing strategies (i.e. UL 94 and ASMT E1354).

Bio:

Ronald Lankone obtained his Ph.D. in Chemistry from Johns Hopkins University, during which time he investigated the degradation and release behavior of nanocomposite materials after natural and artificial weathering. In the fall of 2018, Ron joined the Polymeric Materials Group (PMG) at NIST as an NRC Postdoctoral fellow to study the weathering of home siding materials. Over the last year, Ron has examined changes in siding appearance and performance as a function of artificial UV exposure. He has also initiated fire performance testing of siding materials. As well, Ron has also investigated the weathering of automobile coatings and the mechanical performance of industrial cables after extended periods of accelerated aging.