

Material Matters

The Quarterly Magazine of NIST's Material Measurement Laboratory

Spring 2015

*New Nanosilver Reference Material
Testing Trace Explosive Detectors
Measuring Monoclonal Antibodies*

NIST

National Institute of
Standards and Technology
U.S. Department of Commerce

40 nm



About NIST's Material Measurement Laboratory

The Material Measurement Laboratory (MML) is one of two metrology laboratories within the National Institute of Standards and Technology (NIST). The laboratory supports the NIST mission by serving as the national reference laboratory for measurements in the chemical, biological and material sciences. Our activities range from fundamental and applied research on the composition, structure and properties of industrial, biological and environmental materials and processes, to the development and dissemination of tools including reference measurement procedures, certified reference materials, critically evaluated data, and best practice guides that help assure measurement quality. Our research and measurement services support areas of national importance, such as:

- Advanced materials, from nanomaterials to structural steels to complex fluids
- Energy, from characterization and performance of fossil and alternative fuels to next-generation renewable sources of energy
- The environment, from the measurement of automotive exhaust emissions and other pollutants to assessment of climate change and the health and safety aspects of man-made nanomaterials
- Food safety and nutrition, from contaminant monitoring to ensuring the accuracy of nutrition labels
- Health care, from clinical diagnostics to tissue engineering and more efficient manufacturing of biologic drugs
- Infrastructure, from assessing the country's aging bridges and pipelines to the quality of our drinking water
- Manufacturing, from lightweight alloys for fuel-efficient automobiles to biomanufacturing, advanced electronics, and data for chemical manufacturing
- Safety, security and forensics, from gunshot and explosive residue detection, to ensuring the performance of body armor materials, to DNA-based human identity testing

The Material Measurement Laboratory also coordinates the NIST-wide Standard Reference Materials® (SRM) and Standard Reference Data programs, which include production, documentation, inventory, marketing, distribution and customer service.

The Material Measurement Laboratory is home to more than 900 staff members and visiting scientists at six locations:

- NIST main campus in Gaithersburg, MD
- NIST Boulder Laboratories in Boulder, CO
- Hollings Marine Laboratory in Charleston, SC , where NIST staff work side-by-side with scientists from NOAA, the South Carolina Department of Natural Resources, the College of Charleston, and the Medical University of South Carolina to provide the science, biotechnology and standards needed to understand links between environmental conditions and the health of marine organisms and humans
- Institute for Bioscience and Biotechnology Research (formerly CARB) in Rockville, MD, where scientists from NIST, the University of Maryland College Park, and the University of Maryland School of Medicine conduct research on measurement science and standards issues associated with advanced therapeutics
- Brookhaven National Laboratory in Upton, NY where, in partnership with the Department of Energy, the laboratory has a user facility that enables researchers from industry, academia and other government agencies to apply synchrotron-based x-ray spectroscopy techniques to the development of products like oil additives and next-generation electronics
- The Advances in Biological and Medical Measurement Science (ABMS) Program at Stanford University in Palo Alto, CA, where NIST staff are working elbow-to-elbow with Stanford faculty groups and commercial affiliates to develop standards and tools that enable translation of innovations in quantitative biology and engineered biology to clinical and commercial practice

Cover image: Transmission electron microscopy image of Reference Material 8017 silver nanoparticles deposited onto silica-coated grids. The image shows typical particle morphologies and crystalline nature.

Credit: Thao M. Nguyen, NIST

A Message from the MML Director

At NIST's Material Measurement Laboratory, we work tirelessly to find new ways to measure known substances with ever more precision and accuracy, and measure and characterize new novel substances. An important part of MML's mission is making sure these measurements meet our stakeholders' needs. The wide range of measurement services we provide to our diverse customer base helps ensure that we accomplish this goal.

When clinical labs check the validity of their vitamin D or cholesterol test methods, they are likely to use reference materials developed by scientists at MML. When engineers design new steel bridges and buildings, they are likely to rely on strength tests verified by materials developed at MML. When first responders handle suspicious powders, they are likely to use collection protocols developed at MML.

MML's measurement services include the development of measurement standards—in the form of documented measurement methods, instrument calibrations, and reference materials—that help others generate reliable and reproducible measurements. MML coordinates NIST's Standard Reference Material (SRM) and Standard Reference Data (SRD) programs, including production and distribution of reference materials and data products. SRMs are physical artifacts produced and certified by NIST, and are used by manufacturers and test labs to calibrate instruments, verify the accuracy of measurements and develop new measurement methods. MML-produced Standard Reference Databases (SRDs) are collections of critically evaluated qualitative and quantitative information on the composition, structure and state properties of a variety of substances. NIST provides nearly 1,300 SRMs and 125 SRDs that ensure the accuracy of millions of measurements made daily in medical clinics, manufacturing plants and industrial labs, and federal and state agencies. In this issue of *Material Matters* you can read about a few of them.

Making precise and accurate measurements is only part of what we do at MML. The measurement services we provide ensure that our science is put into practice, and that we continue to meet national needs in the biological, chemical, and material sciences.



Laurie Locascio, Ph.D.
Director, Material Measurement Laboratory
NIST

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New NIST Reference Material Provides a Silver Lining for NanoEHS Research



Credit: Hackley/NIST

NIST's new silver nanoparticle reference material is designed for extended shelf life to support environmental health and safety studies.

Note: A version of this story previously appeared in NIST's TechBeat on March 3, 2015

NIST has issued a new silver nanoparticle reference material to support researchers studying potential environmental, health and safety risks associated with the nanoparticles, which are being incorporated in a growing number of consumer and industrial products for their antimicrobial properties. The new NIST test material is believed to be the first of its kind to stabilize the highly reactive silver particles in a freeze-dried, polymer coated, nanoparticle cake for long-term storage.

Nanoparticulate silver is a highly effective bactericide. It is, by some estimates, the most widely used nanomaterial in consumer products. These include socks and shoe liners (it combats foot odor), stain-resistant fabrics, coatings for handrails and keyboards, and a plethora of other applications.

The explosion of "nanosilver" products has driven a like expansion of research to better understand what happens to the material in the environment. "Silver nanoparticles transform, dissolve and precipitate back into nanoparticles again, combine or react with other materials—our understanding of these processes is limited," says NIST chemist Vince Hackley. "However, in order to study their biological and environmental behavior and fate, one needs to know one is starting with the same material and not some modified or oxidized version.

This new reference material targets a broad range of research applications."

Silver nanoparticles are highly reactive. In the presence of oxygen or moisture they rapidly oxidize, subsequently releasing silver ions. This is the basis for their antimicrobial properties, but it also makes it difficult to create a standardized silver nanoparticle suspension with a long shelf

life as a basis for doing comparative environmental studies. The new NIST product is the first to be stabilized by coating and freeze-drying—a technique commonly used in the pharmaceutical industry to preserve blood products and protein-based drugs. The NIST material uses polyvinylpyrrolidone (PVP), a polymer approved by the Food and Drug Administration for many uses, including as a food additive. The freeze-dried PVP-nanosilver cakes are flushed with an inert gas and sealed under a vacuum. Mixing the cake with water reconstitutes the original suspension.

NIST reference materials are designed to be homogeneous and stable. NIST provides the best available estimates for key properties of reference materials. In this case those include the mean silver particle size measured by four different methods, the total silver mass per vial, and the percentage distribution of nanoparticle sizes. The particles have a nominal diameter of 75 nanometers. NIST expects the material to be stable indefinitely when properly stored and handled, but will continue to monitor it for substantive changes in the reported values.

More information on NIST RM 8017, "Polyvinylpyrrolidone Coated Silver Nanoparticles" is available at https://www-s.nist.gov/srmors/view_report.cfm?srm=8017.

- Michael Baum, NIST

Contact: Vince Hackley, vince.hackley@nist.gov

U.S. Secretary of Commerce Visits NIST at Stanford



Credit: Alex Baker, U.S. Department of Commerce

This February, Department of Commerce Secretary Penny Pritzker (left) visited the NIST Joint Initiative for Metrology of Biology (JIMB) at Stanford University. NIST Director Willie May (right) and MML Director Laurie Locascio joined her during her visit. JIMB is co-led by Stanford University and NIST and is designed to enable significant improvements in the accuracy and comparability of vital data used to make important research, regulatory, clinical, and manufacturing quality control decisions.

Senate Confirms May as 15th NIST Director

Note: A version of this story previously appeared on www.nist.gov on May 5, 2015

On May 4, 2015, the U.S. Senate confirmed Willie E. May as the second Under Secretary of Commerce for Standards and Technology and the 15th director of NIST. May has been serving as acting director since June 2014. He has worked at NIST since 1971, leading research activities in chemical and biological measurement science activities prior to serving as associate director for laboratory programs and principal deputy to the NIST director.

"Willie has been a partner and champion in our efforts to strengthen America's manufacturing sector and promote innovation, key drivers to spurring economic growth, and core pillars of the Department's 'Open for Business Agenda.' In addition to serving as a world-class research institute, NIST has taken the lead on several major Department of Commerce and Obama Administration priorities, including implementing a national network of manufacturing institutes and working with industry and other stakeholders to develop the NIST Cybersecurity Framework," said U.S. Secretary of Commerce Penny Pritzker.

"This honor is something I could never have imagined when I began working as a bench chemist at the National Bureau of Standards more than 40 years ago," said May. "I am fully committed to maintaining NIST as a world-leading scientific research institution providing measurements, standards and technology solutions to our stakeholders. I will work to strengthen our Manufacturing Extension Partnership and Baldrige Performance Excellence programs, which also can significantly contribute to our nation's advanced

manufacturing and innovation goals. I look forward to working with Secretary Pritzker to address the department's new responsibilities called out in the Revitalize American Manufacturing and Innovation Act."

In addition to his responsibilities at NIST, May also serves as the vice president of the International Committee on Weights



NIST Director Willie E. May

and Measures (CIPM) and president of the CIPM's Consultative Committee on Metrology in Chemistry and Biology. May received a B.S. in chemistry from Knoxville College in Tennessee and a Ph.D. in analytical chemistry from the University of Maryland. Before joining NIST (then the National Bureau of Standards), May worked as a senior analyst at the Oak Ridge Gaseous Diffusion Plant. At NIST, his research has focused on trace organic analytical measurement science, the physical and chemical properties of organic compounds and liquid chromatography, which is used to identify the components in a mixture.

Among many other awards and honors, May was elected a Fellow of the American Chemical Society in 2011. He has been

recognized with the Department of Commerce's Bronze (1981), Silver (1985) and Gold (1992) medals. The National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCCHE) has recognized him with both the Percy Julian Award for outstanding research in organic analytical chemistry and the Henry Hill Award for exemplary work and leadership in the field of chemistry. May received the 2007 Alumnus of the Year Award from the College of Chemical and Life Sciences at the University of Maryland, and in 2010 he was among the first class of inductees into the Knoxville College Alumni Hall of Fame. He was the keynote speaker for the 2002 winter commencement ceremonies for the University of Maryland's College of Life Sciences, and for Wake Forest University's Graduate School of Arts and Sciences commencement exercises in 2012.

Credit: NIST

NIST was established in 1901, and since then, has carried out its mission to promote U.S. innovation and industrial competitiveness by making essential contributions to industry, science, public safety and national security. NIST's research and standards development activities cover a broad array of disciplines, from quantum physics to cybersecurity, advanced manufacturing to forensic science.

As a non-regulatory agency of the Commerce Department, NIST promotes U.S. innovation and industrial competitiveness by advancing measurement science, standards and technology in ways that enhance economic security and improve our quality of life. To learn more about NIST, visit www.nist.gov.

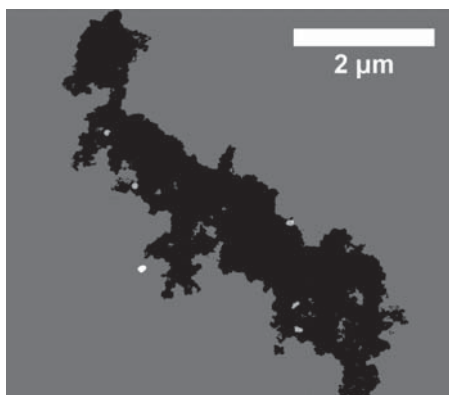
- Jennifer Huergo, NIST

NIST MML Researcher Teams Up with EPA to Study Impact of Fuel-Borne Cerium Oxide Catalyst Nanoparticles in Diesel Fuels

Soot particles emitted by diesel engines have adverse impacts on health and the environment. One solution to address this problem is the use of catalysts to enhance the completion of the fuel combustion reaction, resulting in lower soot emissions. Fuel-borne catalysts such as CeO₂ have been added to diesel fuels for this purpose, and have indeed lowered the soot emissions, especially for the larger soot particles. However, the fate of the CeO₂ particles in the combustion process has not been thoroughly studied. The fuel-borne crystalline CeO₂ particles are in the size range of 4.0 nm to 7.5 nm, and therefore pose health and environmental concerns independent of the soot emissions. In fact, currently CeO₂ additives are only permitted for off-road (i.e., tractors) vehicles in the U.S., although they are approved for on-road use in a number of foreign countries.

Therefore an important question is the history of the CeO₂ nanoparticles after combustion. In the exhaust, do they agglomerate, do they attach to soot particles, or both? Only when this is understood can the potential health and environmental effects of these additives be modeled and studied. In a collaboration with the U.S. EPA, NIST MML researcher Joseph Conny analyzed diesel soot emissions using scanning electron microscopy (SEM) to determine 1) CeO₂ particle size, 2) the extent to which the CeO₂ nanoparticles become attached to soot particles, and 3) the volume that CeO₂ occupies when attached to soot.

Combustion of the diesel fuel took place in a 4.8 kW engine. Particles in several size fractions were collected on polished silicon wafers in a cascade impactor. The quantitative SEM analysis, which involved backscatter electron (BSE) imaging of the CeO₂ and secondary electron (SE) imaging of the soot, took into account the fractal nature of the soot particles to determine its volume fraction; the spherical CeO₂ particles were treated as non-fractal.



Overlay of a BSE image of CeO₂ particles (white pixels) and SE image of a soot particle (black pixels). Five CeO₂ particles are associated with the soot; one CeO₂ particle is unassociated.

Credit: Joseph Conny, NIST

The emitted CeO₂ particles averaged 121 ± 71 nm in diameter. Thus, aggregation of the CeO₂ during combustion resulted in particles that were 16 to 30 times larger on average than the CeO₂ nanoparticles added to the fuel. While most of the CeO₂ particles were attached to large soot particles, 40 % (by number) were not, existing either as individual particles or attached to soot particles smaller than themselves. Among CeO₂ particles that were associated with the large soot particles, the CeO₂ phase accounted for < 1% of the soot particle volume.

Contact: Joseph M. Conny,
joseph.conny@nist.gov

NIST MML Leads Development of ASTM Standard Practice for Testing Trace Explosive Detectors

NIST MML researchers have recently completed development of a soon-to-be promulgated ASTM Standard Practice for testing and scoring the performance of trace explosive detection systems. This standard will be used by instrument developers and manufacturers, testing laboratories, and international agencies responsible for enabling effective deterrents to terrorism. The new standard is an extensive revision of ASTM E2520-07, Standard Practice for Verifying Minimum Performance of Trace Explosive Detectors, which was also developed at MML. The revised Standard Practice goes far in increasing chemical scope, testing levels, realism and practical aspects of explosive screening. A white paper was distributed to outline the expanded tests and metrics and to elicit feedback regarding the performance criteria most important to trace detection. This was followed by interactions with ETD manufacturers, domestic and international agencies, subject matter experts, and stakeholder communities to better define the criteria and formulate a mechanism for scoring ETD performance that was fair and reasonable, technology agnostic, and reflects the most important aspects of trace detection. The revised Standard Practice adapts ASTM Test Method (E2677-14), also developed

through MML, that enables reliable determinations of limits of detection. The revised standard relaxes the requirement that an instrument identify a specific target compound, since some innovative screening technologies cannot do this (such as thermo-energetic detectors and canines), but extra credit is given to those technologies that can provide identification. The revision requires the use of a standard background challenge material, such as a natural dust or dirt ("standard schmutz") that represents the matter co-collected on swabs during the process of sampling. For this purpose, pertinent NIST natural matrix Standard Reference Materials are identified. Because sample throughput is important at security checkpoints, the measurement of average throughput rate for background-loaded samples is required. Lastly, the revised Standard Practice provides a means to calculate a numerical performance score based upon all the mandated tests. There is no maximum score but a minimum score is specified based upon criteria from the original E2520-07. The scores will provide tangible measures of instrumental detection performance, useful for comparing systems worldwide and for enabling targeted improvements in next-generation detection systems.

Contacts: Mike Verkouteren,
r.verkouteren@nist.gov
Greg Gillen, j.gillen@nist.gov
William MacCrehan,
william.maccreehan@nist.gov

Understanding Biomass Thermodynamic Properties

Cellulose is everywhere – in trees, grass, shrubs, and paper. In fact, it is the most abundant organic polymer on Earth. Due to the ubiquity of cellulose and its widespread use in applications such as the conversion of cellulose biomass to glucose, ethanol, and other useful chemicals, there is a great deal of interest in understanding its properties. Recently, scientists from NIST, the National Renewable Energy Laboratory (NREL), Brigham Young University, and the University of Porto in Portugal undertook a collaborative effort to measure the thermodynamic properties of cellulose. The study has led to calculated values that are fundamental to bioprocess engineering and can be used to predict the energy relationships in any reaction or process involving the cellulose allomorphs, including the utilization of cellulose for renewable energy applications and cellulose photosynthesis.

Chemically, cellulose is a polymer made up of a linear chain of several hundred to several thousand connected D-glucose molecules. It has been known for many years that naturally occurring cellulose

can be chemically changed into other allomorphs that have essentially the same chemical backbone but differ in their hydrogen bonding patterns and in glucose conformation. Understanding the thermodynamic properties of these allomorphs is essential for calculating the energy requirements and position of equilibrium for any process in which cellulose participates.

To conduct their research, the collaborative team measured the thermodynamic properties, i.e., massic heat capacities from 2 K to ambient temperature, massic enthalpies of solution in the solvent cadoxen, and massic enthalpies of combustion in oxygen of NREL prepared and well-characterized cellulose allomorphs by using heat capacity, solution and combustion calorimetry. Obtaining



thermodynamic properties is challenging because the allomorphs are in fact mixtures with amorphous cellulose and bound water, both of which need to be accounted for. The problem was solved by using X-ray diffraction to measure the fractions of crystalline cellulose in each of the samples and by using thermodynamic data from the literature on the massic enthalpy of wetting of the cellulose allomorphs. By using the data resulting from this study in combination with other established property values, the team calculated additional thermodynamic properties such as the massic enthalpy, entropy, and Gibbs energy of formation. As a result, this study* contains the most extensive set of thermodynamic property values for the cellulose allomorphs to date.

*R.N. Goldberg, J. Schliesser, A. Mittal, S.R. Decker, A. Filipa L.O.M. Santos, V.L.S. Freitas, A. Urbas, B.E. Lang, C. Heiss, M.D.M.C. Ribeiro da Silva, B.F. Woodfield, R. Katahira, W. Wang, and D.K. Johnson, A thermodynamic investigation of the cellulose allomorphs: cellulose(am), cellulose Ib(cr), cellulose II(cr), and cellulose III(cr), *The Journal of Chemical Thermodynamics*, 81 (2015) 184-226. DOI: <http://dx.doi.org/10.1016/j.jct.2014.09.006>
Contact: Robert Goldberg, robert.goldberg@nist.gov

Neutron Diffraction Reveals Structural Interactions of a Voltage Sensor Toxin with Lipid Membranes

A variety of toxins from venomous animals are known to alter the activity of diverse ion channel proteins including voltage, stretch, and ligand-activated cation channels. In vivo, the opening and closing of ion channels to ion conduction across cellular membranes (channel gating) is regulated by the membrane polarity and interactions between the channels and small molecules. Medical conditions that affect the central and peripheral nervous systems are caused by dysfunction of ion channel proteins, in particular voltage-gated (Kv) ion channels. Understanding how channel activities are altered by the interactions with small molecules has significant implications for the treatment of cardiac and neuronal disorders. The voltage-sensor toxin VSTx1 from tarantula

venom is a small protein known to bind to voltage-sensitive domains of Kv channels and to modify their gating mechanism. Although tarantula toxins have been shown to partition into membranes, and the membrane is thought to play an important role in their activity, the structural interactions between these toxins and lipid membranes are poorly understood.

A team of researchers from the NIST/University of Maryland-led Institute for Bioscience and Biotechnology Research, National Institutes of Health and University of California, Irvine have examined the molecular details of the interactions of the VSTx1 toxin with lipid membranes. The team produced active forms of the VSTx1, carrying stable deuterium isotopes, from its synthetic, linear form, and tested its inhibitory function against Kv channels expressed in oocyte membranes using voltage-clamp techniques. By using a combination of solid state NMR spectroscopy and neutron diffraction on VSTx1 incorporated into model lipid membranes, the study revealed to what

extent the tarantula toxin influences the structure and dynamics of the lipid bilayer. Deuteration schemes of the toxin and the lipid, in conjunction with neutron diffraction methods, showed that the toxin partitions interfacially in the membrane and distorts the membrane to produce thinning and increased disorder of the hydrocarbon core. Molecular modeling of neutron data with deuterium contrast chosen to highlight a particular region on the surface of the toxin, that is thought to be implicated in binding to the voltage sensors, demonstrated that the VSTx1 toxin adopts a preferred orientation, exposing the binding surface laterally in the membrane so as to facilitate formation of the toxin-channel complexes. The results of this study have been published online and in print by the *Proceedings of the National Academy of Sciences*: December 1, 2014, doi:10.1073/pnas.1415324111 PNAS December 16, 2014 vol. 111 no. 50 E5463-E5470.

Contact: Ella Mihaiulescu, ella.mihaiulescu@nist.gov

NIST Facility for Adsorbent Characterization and Testing (FACT)

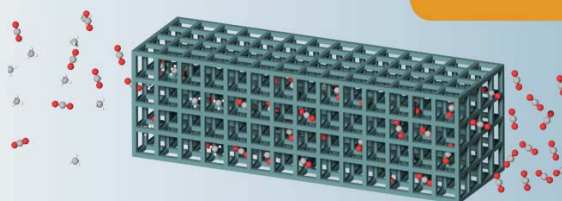
ENERGY

Objective

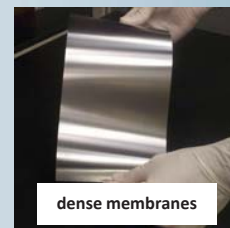
Adsorbent materials have many applications related to sustainable development, including hydrogen and methane storage, gas separation, catalysis, methane conversion, and natural gas purification.

While advances are being made, the pace of innovation is significantly slowed by a lack of reproducibility in sorption isotherm measurements, particularly at high pressure, due to a lack of standardized protocols and sample activation methods.

FACT supports programs developing adsorbents and serves the sorbent materials research community by providing impartial testing and characterization of material sorption properties, establishing testing procedures, and disseminating sorbent material property data and measurement best practices.



powders, porous solids



dense membranes

Impact and Customers

SEPARATION



Greenhouse Gas Mitigation:

For example, accelerated discovery of cost-efficient materials for CO₂ separation from natural gas calls for fundamental understanding of gas sorption mechanisms in the presence of competing species.

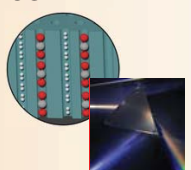
STORAGE



Fuels:

For example, the rational design of materials for on-board CH₄ or H₂ storage requires the optimization of the sorption kinetics in nanovalved adsorbents for efficient adsorption and release.

CONFINEMENT



Photonics:

For example, advancing technology to modulate the frequency of high intensity lasers requires the study of gas-filling properties in hollow-core crystal fibers.

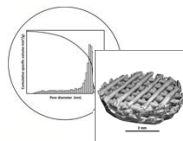
CONVERSION



Gas-to-Liquid:

For example, innovation in biomimetic catalysts for the conversion of methane to liquid fuels or others added-value chemicals demands data on interactions between reactant, products, and catalyst surface.

POROSIMETRY



Additive Manufacturing:

For example, design optimization of porous 3D printed materials (hierarchical mesoporous bioactive polycaprolactone scaffolds, cathodes/anodes for lithium-ion microbatteries, lightweight cellular solids for aviation) requires high resolution pore analysis.



Approach

To address the challenges inherent to measuring sorption properties, NIST with support from the U.S. Department of Energy's Advanced Research Projects Agency-Energy (ARPA-E) has recently commissioned a state-of-the-art laboratory, the Facility for Adsorbent Characterization and Testing (FACT), with the goal of establishing an independent laboratory for accurate and reliable characterization of gas sorption properties of materials.

FACT houses instruments for characterizing the pore architecture and evaluating fundamental sorption properties of materials upon exposure to single gases, binary gas mixtures, and multicomponent gas mixtures. These instruments will be used to generate reliable gas sorption isotherms.

FACT researchers will develop and standardize protocols for activating samples prior to gas sorption experiments and establish best practices for high pressure sorption isotherm measurements. An existing NIST reference material (RM-8852, Ammonium ZSM-5) will be evaluated for the measurement of reference data, specifically CO₂ and CH₄ sorption isotherms.

Facility Description

Five state-of-the-art instruments, with complementary measurement capabilities, are installed in the FACT lab. A summary of the performance characteristics for these instruments is given in Table 1. The instruments use different measuring principles, making it possible to cross check results. The availability of complementary measurement technologies in a single laboratory and capability to measure adsorption propensities in gas mixtures makes this laboratory a unique venue capable of measuring reference data and exploring the frontiers of adsorption science.

Volumetric

The four-channel volumetric gas sorption instrument covers a wide range of pressures. Channel 2 features a small sample holder (0.5 cc) with a reduced dead volume, for reliable isotherm measurements on small samples.



Figure 1. Combined tool for binary gases. A magnetic suspension balance monitors mass uptake without contact between the sample holder and measuring instrument.

Table 1. List of state-of-the-art instruments in the FACT lab

Instrument		P range	T range	AST***	Static	Flow
Volumetric	Ch1*	0 bar – 200 bar	78 K – 780 K	Yes	Yes	-
	Ch2	0 bar – 80 bar	20 K – 670 K	Yes	Yes	-
	Ch3*	0 bar – 1 bar	LN ₂ , LAr, RT – 670 K	Yes	Yes	-
	Ch4*	0 bar – 100 bar	RT – 670 K	Yes	Yes	-
Gravimetric*		0 bar – 20 bar	273 K – 773 K	Yes	Yes	Yes
Volumetric & Gravimetric		0 bar – 90 bar**	LN ₂ , LAr, 273 K – 423 K	-	Yes	-
Volumetric with chromatography		0 bar – 90 bar**	283 K – 670 K / 283 K – 323 K	Yes	Yes	-
Pore size analyzer (volumetric)		0 bar – 1 bar	RT – 670 K / LN ₂ , LAr, 253 K – 373 K	Yes	Yes	-

*: Mass spectrometry available for gas analysis.

** : Higher pressure measurements are possible for single gas sorption isotherms.

***: Air-less sample transfer capability.

Gravimetric

The gravimetric gas sorption analyzer has an ultrasensitive, temperature-controlled microbalance, providing high resolution and signal stability. The instrument can measure sorption isotherms in either static or dynamic flow mode.

Pore Size Analyzer

The low pressure volumetric gas sorption instrument measures surface area and pore size distributions, and includes a 0.1 torr transducer for high-resolution micropore analysis.

Combined Tools

The combined gravimetric/volumetric instrument can measure sorption isotherms of binary gas mixtures. A second volumetric instrument, equipped with a gas chromatograph, can measure sorption isotherms for multicomponent gases.



Figure 2. Continuously vented cabinets for hydrogen and methane gas cylinders



Figure 3. Combined Tools: Sorption isotherm measuring station for binary gas mixtures (bottom right) and volumetric tool with gas chromatography for multicomponent gases (upper left).

Learn More

Brad Boyerinas, Jarod Horn, Roger van Zee, Marty Green, Carlos Gonzalez, John Small

Laura Espinal
301-975-8979
laura.espinal@nist.gov

www.nist.gov/FACT

Publications

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Using Concatamers as Internal Standards for Quantifying Proteins

Proteins, known collectively as the proteome, represent one of the most complex aspects of our biological machinery. A single protein can serve a number of different functions depending upon particular modifications that occur after protein biosynthesis. Hence, research into biological processes and their disease-related changes often requires the measurement of multiple protein forms of interest in complex biological samples such as blood or tissues. Although there are many different methods for qualitatively evaluating the proteome, mass spectrometry has emerged as a key platform for quantifying proteins. Quantification of proteins typically involves the use of enzymes such as trypsin to break the protein into smaller fragments (peptides) that are more readily analyzed by mass spectrometry. Trypsin cleaves the protein into peptides in a predictable manner at specific amino acid sequences. A mass spectrometry technique known as multiple reaction monitoring (MRM) is then used to focus on quantification of peptides that correspond to a protein or set of proteins of interest.

Quantification in mass spectrometry is often based upon comparing the signal for the molecule of interest to that of an internal standard added in a known amount. The ideal internal standard is chemically and structurally similar to the analyte, and stable-isotope labeled versions of the analyte serve this purpose. Production of isotopically labeled versions of proteins, however, is not

always feasible. Alternatively, stable isotope-labeled synthetic peptides are broadly available. A potential drawback of using peptides as internal standards to measure proteins is that the accuracy of the MRM method can be compromised if incomplete trypsin digestion of the target protein occurs. A third approach involves generation of an artificial protein comprised of linked (concatenated) peptides from the protein or proteins of interest. These quantification concatamers (QconCATs) are simpler to produce than labeled proteins but are cleaved by trypsin in much the same manner as native proteins. One potential limitation of direct concatenation is that natural amino acid sequences surrounding the sites of trypsin-catalyzed cleavage are not identical in the QconCAT and the target proteins. NIST MML researchers have recently examined the impact of these amino acid sequences on quantification accuracy and the results are highlighted in two recent publications*,**. Experiments reveal that at least 6 amino acid residue natural flanking sequences for each Q-peptide are required for reliable quantification.* With appropriate optimization, it appears that QconCATs can avoid the intrinsic limitations of recombinant proteins and synthetic peptides and can be recommended as simply available multiplexed internal standards for protein quantification in MRM assays.

* C. S. F. Cheung, K. W. Anderson, M. Wang, and I. V. Turko, *Anal. Chem.* 2015, 87, 1097-1102.

** J. Chen and I.V. Turko, *Trends in Anal. Chem.* 2014, 57, 1-5.

Contact: Larik Turko, illarion.turko@nist.gov

Particle Shape Effects on Subvisible Particle Sizing for the Biopharmaceutical Industry

The presence of "subvisible" (2 mm to 100 mm) protein particles in biopharmaceuticals can give rise to unwanted immunogenic response. These particles can form as a result of thermal, mechanical, or chemical stress combined with interactions with surfaces or interfaces in the container or associated with non-biologic particles in the drug substance. Measurement of the size distribution of these particles has become an important challenge for industry and regulatory entities. Particle analysis tools for the subvisible size range, such as Light Obscuration (LO), Flow Imaging (FI), and Electrical Sensing Zone (ESZ), often produce results that do not agree with one another. This is despite their general agreement when characterizing polystyrene latex spheres that are supplied with the instruments for calibration. Based on the observation that particles that form in biopharmaceuticals are generally not spherical, but have variable shapes, NIST MML researchers produced test particles of precisely controlled shape (rods and disks) using microlithography. These particles were used with commercial instruments to test the influence particle shape has on measured results. A microfluidic system that combines measurement techniques was developed to further elucidate the differences. Computer models were used to calculate expected ESZ signals. Though the microfabricated particles are highly monodisperse, the commercial instruments produce broadened peaks, and report mean size parameters that are different for different instruments. The microfluidic system helped to clarify the effects of flow alignment and tumbling on the measurements. Effects of imperfect focus and diffraction on imaging results were clarified and a correction algorithm was presented that reduces discrepancies for rod-shaped particles. The results will be useful for researchers and biomanufacturers that use these techniques to characterize subvisible particles. This work is now available in print* and download at the *Journal of Pharmaceutical Sciences* (<http://onlinelibrary.wiley.com/doi/10.1002/jps.24263/abstract>).

* Cavicchi, R. E., et al. (2015). "Particle Shape Effects on Subvisible Particle Sizing Measurements." *J Pharm Sci* 104: 971-987.

Contact: Richard Cavicchi, richard.cavicchi@nist.gov

New Quantitative Image Analysis Software Released

Nathan Hotaling and Carl Simon Jr. of NIST MML's Biomaterials Group have developed an open source plugin, called DiameterJ, which can quantify metrics about fibrous structures in images. The plugin is used with a free, open source, image analysis package, originally developed by the NIH, called ImageJ. They have validated the software using both digital synthetic images and real SEM images of metal wire with well-defined diameters. The software is compatible with many different image segmentation algorithms and is easily incorporated into other analysis packages to encourage use by the community. Hotaling and Simon created a webpage on the ImageJ website with an in-depth explanation of how to use DiameterJ, how it works, and the source code: <http://imagej.net/DiameterJ>.

Contacts: Nathan Hotaling, nathan.hotaling@nist.gov;
Carl Simon Jr., carl.simon@nist.gov

NIST MML Develops NMR 'Fingerprinting' for Monoclonal Antibodies

Note: A version of this story previously appeared in NIST's TechBeat on April 14, 2015

NIST MML researchers at the Institute for Bioscience and Biotechnology Research (IBBR) have demonstrated the most precise method yet to measure the structural configuration of monoclonal antibodies (mAbs), an important factor in determining the safety and efficacy of these biomolecules as medicines. Monoclonal antibodies are proteins manufactured in the laboratory that can target specific disease cells or antigens (proteins that trigger an immune reaction) for removal from the body. The method described in a recent paper* may soon help manufacturers and regulators better assess and compare the performance and quality of mAbs.

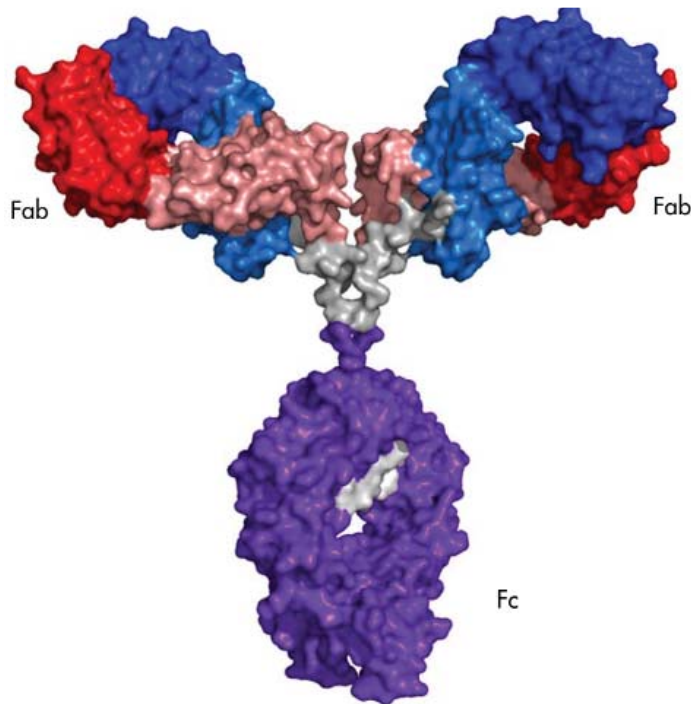
The IBBR is a joint institute of NIST and the University of Maryland.

Monoclonal antibodies can be used as extremely specific therapeutic agents, including ones designed to target cancer cells unique to an individual. However, in order to properly function as a biotherapeutic agent, the molecule's structural units—amino acids—must fold into a three-dimensional structure that aligns its active regions with corresponding receptor sites on a target cell or antigen. If misfolding occurs, a potent and safe treatment may become ineffective, or worse, provoke a dangerous or fatal immune reaction. High-resolution spectral analysis—imaging at the atomic level where even the bonds between hydrogen and carbon atoms are distinguishable—is required to precisely define the mAb's structure and determine if the protein is folding properly.

"We refer to this as 'measuring fingerprints,' because just as a person has

a unique set of fingerprint patterns, each mAb has a one-of-a-kind spectral makeup," says NIST research chemist Robert Brinson. "If we can map that spectral fingerprint, we can determine whether or not folding is occurring as desired."

To do this, the IBBR team turned to a solution that would surprise most biopharmaceutical experts: two-dimensional nuclear magnetic resonance (2D NMR) spectroscopy. NMR is a technique that measures the atomic signature of



A schematic showing the NISTmAb monoclonal antibody, an immunoglobulin G (IgG) molecule being developed by NIST as a reference material. The labels mark the fragments Fab and Fc that were used in the novel NIST two-dimensional NMR fingerprinting method to measure the structural configuration of the entire antibody. Credit: NIST

a molecule similar to how doctors use magnetic resonance imaging (MRI) to noninvasively view organs. "To date, it's been assumed that 2D NMR could not be practically applied to monoclonal antibodies because it's too insensitive, too time intensive and too expensive for analyzing anything other than much smaller drug molecules," Brinson explains.

In pushing the boundaries of the technique, the IBBR team used an NMR system with a high magnetic field strength to produce the first 2D NMR map of a complete, drug-like mAb.** The map was generated using signals from methyl groups.

"Methyl groups are dispersed throughout the mAb structure and, in particular, in the folded cores of the molecule that we want to evaluate," Brinson says. "We can use their signals to yield a specific spectral fingerprint that reflects the unique structure of the mAb."

To make the 2D NMR method more accessible to the lower-strength magnetic field instruments found in most analytical research labs, the IBBR team narrowed the analysis by dividing its sample antibody into two structural fragments. "We mapped the 2D NMR signals generated by the subset of methyl groups found in these fragments, both about a third of the size of the entire protein," Brinson says. "The sum of the data gained from this analysis was found to be a good proxy for the spectral fingerprint of the full mAb."

The new 2D NMR fingerprinting method also overcomes the problems of cost and time. "We reduced the time needed for our measurements from many hours to about 30 minutes," Brinson says.

Brinson says that he and his colleagues are now working on a statistical method that will allow users of their 2D NMR methodology to compare fingerprints from multiple protein samples. "With that ability, manufacturers will be able to quantitatively show that spectra obtained from different lots of the same drug product are identical, enabling them to

better meet regulatory requirements for quality and performance," he says.

* L.W. Abrogast, R.G. Brinson and J.P. Marino. Mapping monoclonal antibody structure by 2D ¹³C NMR at natural abundance. *Analytical Chemistry*, 87: 3556-3561 (2015). DOI: 10.1021/ac504804m

** The monoclonal antibody used in this experiment is NISTmAb, an immunoglobulin G type 1 donated by MedImmune and being developed by NIST as a reference material.

- Michael Newman, NIST

Contact: Robert Brinson, robert.brinson@nist.gov

NIST MML Promotes Careers in Science for Underrepresented and Minority Groups at Scifest Africa

Jeanita Pritchett of NIST MML's Organic Chemical Measurement Science Group was recently awarded a 2014/2015 U.S. Embassy Science Fellowship to provide outreach to minority and underrepresented groups in South Africa. During her three-month internship, she developed and presented interactive workshops for learners in the Grahamstown area to promote awareness and enthusiasm about careers in science. She was influential in promoting chemistry at Scifest Africa, South Africa's National Science Festival. She worked with Scifest organizers to develop the Scifest Africa Workshop Programme and assisted with the planning and implementation of the Etcetera Programme for the festival. These programs and workshops were attended by over 64,000 people and offered hands-on activities that afforded participants opportunities to immerse themselves in the practice of science. One of the workshops that she developed, Foam Gnomes: Understanding Chemical Changes, was awarded "Best workshop: Curriculum" at this year's festival.

Scifest Africa 2015 celebrated the International Year of Light. The theme explored a number of sub-themes including, but not limited to, anatomy, architecture, arts and culture, astronomy, atmospheric sciences, aviation, biotechnology, chemistry, diet, energy, fiber optics, gravity, lasers, matter, microscopy, nanotechnology, optics, photonics, space sciences, the spectrum, and the universe. These topics were represented through a number of hands-on, interactive activities, workshops, and lectures. Pritchett served as a Logistics Officer by coordinating over 100 events throughout the festival. Additionally, Pritchett spoke to a number of attendees during her invited lecture about what NIST's missions are, potential careers, ways to diversify the STEM field, and a variety of funding opportunities.

Outside of the festival, Pritchett also served as an Outreach Officer. There is a large demand to take science to learners, educators, and communities who cannot afford to attend the festival or simply don't have the resources to successfully teach STEM projects. Pritchett and her outreach team organized a number of outreach tours to local and rural schools in the Eastern Cape. The goal was to increase awareness about the STEM fields and to enhance their learning process. When surveyed, a majority of STEM educators for grades 7-12, stated that they were inadequately trained to be able to effectively teach their subject. As an effort to combat this, Pritchett led several workshops for educators at the Nelson Mandela Bay Science and Technology Centre (Uitenhage, South Africa) geared at showing them innovative ways to teach their respective subjects. Overall the programs that Pritchett implemented were well received and will be continued to be used during festivals in the future.

The Embassy Science Fellows Program provides U.S. embassies access to the expertise of U.S.

Government officers in science and technology fields. U.S. Embassies request Fellows to assist on science, technology, environment, or health issues. They recommend projects that will have significant positive impact on their host countries and our bilateral relationship. The work of Embassy Science Fellows has contributed to policy development and collaboration with host governments, universities, and other organizations.

Contact: *Jeanita Pritchett, jeanita.pritchett@nist.gov*

Vol. One of Therapeutic Monoclonal Antibody Characterization Book Series Published by ACS

A large scale collaboration with biopharmaceutical industry stakeholders came to fruition in December 2014 with the publication of Volume 1 of "State-of-the-Art and Emerging Technologies for Therapeutic Monoclonal Antibody Characterization" (<http://pubs.acs.org/isbn/9780841230262>). The first volume in the series, "Monoclonal Antibody Therapeutics: Structure, Function, and Regulatory Space," provides an industry-driven discussion of this critical therapeutic class, their regulatory considerations, and the role reference materials may play in biopharmaceutical development. Notable pioneers in the field contributed chapters on development of protein therapeutics and biochemical functions essential to their therapeutic efficacy for treating diseases such as cancer and autoimmune disorders.

The book series, co-edited by John Schiel (NIST-MML), Darryl Davis (Janssen), and Oleg Borisov (Novavax), is based on the NISTmAb Reference Material to be released later this year. The second and third books in the series contain materials, methods, and data for the NISTmAb that collectively represent the current and emerging characterization toolbox. Throughout this effort, a first-of-a-kind repository of regulatory considerations, experimental methods and data, and a widely available reference mAb for future technological development will be available to industry, academic researchers, regulatory agencies, and instrument manufacturers. The series will contain six chapters authored by NIST scientists that span multiple divisions contributing to the NISTmAb development effort.

Contact: *John Schiel, john.schiel@nist.gov*

NIST MML Researchers Evaluate Stable-Isotope Labeled Internal Standards for Protein Quantification

Researchers from NIST MML's Bioanalytical Science Group have systematically compared several platforms for stable-isotope labeled internal standards that can be used to quantify proteins in biological samples. Protein quantification based on stable-isotope labeling mass spectrometry (SIL-MS) involves adding known quantities of stable-isotope labeled internal standards into biological samples. The internal standards are analogous to native molecules and quantification is achieved by comparing signals from isotope-labeled and native molecules. This methodology is broadly applicable and used to measure clinical biomarkers which require accurate and precise protein abundance measurements. Several internal standard platforms exist for protein quantification; however there are few comparisons of performance (accuracy, precision, and robustness) between the different approaches.

The NIST group compared several internal standard platforms and evaluated the performance of each to accurately quantify three clinically relevant, model human proteins. The platforms compared included full-length recombinant human proteins, synthetic peptides, and QconCATs (Quantification concatamers). A QconCAT is a series of concatenated peptides (corresponding to multiple proteins) resulting in a synthetic protein. Multiple versions of the synthetic peptides and QconCAT were assessed. These versions included natural flanking sequences to make the internal standard better mimic the target, endogenous molecule to be quantified. For each approach, protein quantification based on ten individual peptides was assessed. These peptides differ in mass, hydrophobicity, enzymatic digestion kinetics, and digestion efficiency to evaluate the performance of these platforms when both optimal and non-optimal performing proteotypic peptides are used for protein quantification. This study provides researchers with insight on the performance of several internal standards in terms of accuracy and robustness.

Reference: Scott, K. B., Phinney, K. W., and Turko, I. V., Quantitative Performance of Internal Standard Platforms for Absolute Protein Quantification using Multiple Reaction Monitoring Mass Spectrometry, Analytical Chemistry, Available online 26 March 2015, <http://pubs.acs.org/doi/abs/10.1021/acs.analchem.5b00331>.

Contact: *Kerry Scott, kbauer@ibbr.umd.edu*

ADA Foundation Names New Director for the Dr. Anthony Volpe Research Center

The ADA Foundation (ADAF) has named Dr. Thomas C. Hart as the new director of the ADAF Dr. Anthony Volpe Research Center (VRC). His tenure at the helm of the VRC began April 2, 2015.

A distinguished scientist, academic, researcher and mentor, Dr. Hart previously served as professor of periodontics and director of Craniofacial Population Sciences Research at the University of Illinois at Chicago College of Dentistry and he presently serves as the chair of the American Dental Association (ADA) Council on Scientific Affairs. He earned a B.A. in biology from the University of Virginia, a D.D.S. degree from Emory University in Atlanta, and a Ph.D. in human genetics from Virginia Commonwealth University.

In addition to his academic and research experience, Dr. Hart has clinical experience as a practicing dentist (periodontist) in one of the largest dental practices in North Carolina. Previous positions included the National Institute of Dental and Craniofacial Research in the National Institutes of Health, where he served as chief of the Human Craniofacial Genet-



Thomas C. Hart

ics section of NIDCR from 2003 to 2010, and as clinical director of that same institute from 2003 to 2008. He was also an Associate Professor at the University of Pittsburgh School of Dentistry. His present research focuses on understanding genetic determinants of diseases of the craniofacial region, with the goal of improving diagnosis and treatment. He is the author of more than 150 scientific publications. Dr. Hart has been successful in securing a number of NIH grants, either as a sole investigator or as a collaborative investigator.

With his proven ability to secure outside funding, previous chairmanships and teaching experience, he will serve the ADA Foundation and the Volpe Research Center well as a director, mentor and a guide to develop an innovative research program. Formerly known as the Paffenbarger Research Center, the Dr. Anthony Volpe Research Center laboratory facility is operated by the ADA Foundation and is located on the Gaithersburg campus of NIST, embedded within the Biosystems and Biomaterials Division. The ADA Foundation and NIST have had a CRADA since 1928. Previously operated by the ADA as the Research Unit and then jointly by the ADA and the ADA Foundation, the original mandate was to develop standards and test methods for dental materials that would provide for consistency, performance and safety, which in turn would benefit the dental profession and the public. After developing many products that are currently used by dentists and physicians worldwide, the lab continues its dental materials research program and also conducts unique research in cutting-edge fields of biomaterial and tissue engineering technologies, tissue regeneration, molecular biology and microbiology.

Contact: Gary Schumacher,
gary.schumacher@nist.gov

U.S. Patent Issued to NIST MML Biomolecular Measurement Team

The U.S. Patent and Trademark Office (PTO) has granted NIST a patent on a method of characterizing glycans, complex chains of sugar molecules that are attached to glycoproteins. Many therapeutic proteins such as monoclonal antibodies are glycosylated and rapid methods for characterizing glycans are needed in manufacturing to ensure consistency of these glycoprotein products. The newly issued U.S. Patent No. 8,962,345, "Method of Characterizing Glycans attached to Glycoproteins," describes a method for rapid glycan characterization and includes the following steps. First, the glycoproteins are sponta-

neously immobilized on colloidal particles such as gold nanoparticles forming glycoprotein/colloidal particles. It is thought that the adsorption of the glycoproteins promotes protein unfolding and presentation of the relatively hydrophilic glycans to the surrounding aqueous solution. Another protein called a lectin is then added to the solution. Different lectins can recognize and bind glycans reversibly and with high specificity. In addition, each lectin molecule contains two or more carbohydrate-combining sites, i.e., they are di- or polyvalent. Therefore, when an appropriate lectin is added to a solution containing the glycoprotein/gold colloid conjugates, the lectin recognizes and binds the oligosaccharides that project out from the surface and cause cross-linking of the glycoprotein/gold colloid conjugates. Because the optical properties of the

gold colloids are sensitive to interparticle separation distance, cross-linking leads to a change in color or scattered light that is detected visually or with optical methods.

The goal of this patented work was to develop a simple, rapid, method for glycan identification that could be used for industrial bioprocess monitoring applications involving glycosylated therapeutic proteins. The inventors are Rebecca Zangmeister and Mike Tarlov from MML and two former NRC postdoctoral fellows, Germarie Sanchez-Pomales and Todd Morris.

Contact: Rebecca Zangmeister, rebecca.zangmeister@nist.gov

Outreach and Partnering

NASA and NIST Sign Memorandum of Understanding for Materials Research on the International Space Station

NASA and NIST have signed a memorandum of understanding to collaborate during the “MaterialsLab” program of materials research for the International Space Station (ISS). This agreement will leverage the expertise of the two agencies in materials measurements, processing, analysis, data, and modeling to enhance the impact of ISS microgravity research. This collaboration will also provide benchmark data for evaluating and improving Materials Genome Initiative models for the microstructure and properties of materials. NASA Administrator, Charles F. Bolden and NIST Director Willie E. May signed the agreement in March of 2015. *Contact: Richard E. Ricker, richard.ricker@nist.gov*

2nd Cell Manufacturing Workshop Held to Advance Roadmap

The second facilitated Cell Manufacturing Consortium (CMC) workshop was held February 27th at NIH in Bethesda, Maryland. The Georgia Research Alliance and Georgia Institute of Technology received funds from the NIST Advanced Manufacturing Technology Consortia (AMTech) program to develop an industry roadmap that aims to provide a pathway to overcome cell manufacturing industry challenges and capitalize on opportunities that will maintain the United States' position at the head of the rapidly expanding global cell manufacturing industry. The workshop was attended by approximately 60 experts from academia, industry, and government agencies to generate information that will form the basis of a Cell Manufacturing Roadmap.

Contact: Sheng Lin-Gibson, sheng.lin-gibson@nist.gov

NIST Holds Annual Biopharmaceutical Measurement Roundtable

NIST staff scientists met with key members of the biopharmaceutical industry on January 28, 2015 in Washington, DC to discuss key technical gaps involved in the manufacturing of biologic medicines. This is the 4th year in a row that NIST has held the Biopharmaceutical Measurement Roundtable, which is held in conjunction with the Well-Characterized Biological Products Conference held annually in Washington. NIST has initiated a major program in biologic medicines and the purpose of the Roundtable is to ensure that NIST's program is addressing current high priority measurement problems confronting the entire industry and to identify future ones. *Contact: Michael Tarlov, michael.tarlov@nist.gov*

NIST Hosts U.S. Biotech Technical Advisory Group Meeting

NIST MML and the NIST Standards Coordination Office hosted the 3rd Plenary and Working Group Meetings of the U.S. Technical Advisory Group (TAG) to ISO/TC 276 Biotechnology on March 16-17, 2015. Meeting participants included USG (NIST, State, FDA, NIH, USDA), NGO (Alliance for Regenerative Medicine, College of American Pathologists, International Society for Cellular Therapy), and key industry stakeholders. The primary focus was to advance critical standards to enable international research cooperation and commerce for emerging biotechnology sectors.

Contact: Sheng Lin-Gibson, sheng.lin-gibson@nist.gov

Recent NIST MML Awardees

MML Chemical Engineer Inducted into Missouri S&T Academy of Chemical Engineers

Allan Harvey, a member of NIST MML's Theory and Modeling of Fluids Group was inducted into the Academy of Chemical Engineers of the Missouri University of Science and Technology on April 16 (his undergraduate alma mater; formerly the University of Missouri-Rolla). The Academy recognizes graduates “who have provided outstanding leadership, attained significant levels of professional achievement and success, and demonstrated high standards of personal and professional integrity.” Harvey's research focuses on applying molecular theory to the prediction and correlation of fluid thermophysical properties.

NIST Emeritus Fellow Boettinger Receives 2015 William Hume-Rothery Award

Dr. William Boettinger, NIST MML Emeritus Fellow, received the 2015 William Hume-Rothery Award for outstanding contributions to thermodynamics and kinetics of metallurgical systems and their application to the understanding of alloy microstructures and the relationship to processing conditions at this year's Minerals, Metals, and Materials (TMS) Annual Meeting. This award recognizes a scientific leader for exceptional scholarly contributions to the science of alloys by inviting the winner to present at the William Hume-Rothery Memorial Symposium.

NIST MML Biomedical Engineer Justin Zook Selected as CCR Rising Star

NIST MML biomedical engineer Justin Zook has been selected by the Council for Chemical Research 2015 Annual Meeting program committee to be part of a select group presenting at the RISING STAR poster session. Zook's recent work developing reference materials, methods, and data for the human genome has changed the outlook for broad adoption of clinical sequencing. These reference materials are the first of their kind, and the first class of materials characterized for such a large set of parameters.

Munson Named 2015 SynBio LEAP Fellow

NIST MML researcher Matthew Munson has been named a 2015 SynBio LEAP Fellow. Following a successful pilot, the Synthetic Biology Leadership Excellence Accelerator Program (SynBio LEAP) recently announced 23 Fellowships awarded to an outstanding group of next generation leaders competitively selected for their visions and aspirations for shaping biotechnology for the public good.

Atencia Wins Innovation, Invention Awards

Javier Atencia, a member of NIST MML's Bioassay Methods Group and a University of Maryland Assistant Professor, won the Best Inventor Pitch at the UMD Professor Venture Fair this past November. Javier's novel technique to detect pathogens in food was one of five selected to be presented to a team of regional venture capitalists and entrepreneurs. Atencia was also named the recipient of the UMD Office of Technology Commercialization Invention of the Year Award for the Life Science category. Atencia was recognized for his work developing a chip used to separate bacteria from complex food samples.

Selected Recent Publications

MML researchers publish over 400 journal articles each year. Here are a few recent examples:

- F. W. DelRio, R. F. Cook, B. Boyce, "Fracture strength of micro- and nano-scale silicon components" *Journal of Applied Physics*, (13-May-2015) (PubID: 917944)
- K. W. Anderson, I. V. Turko, M. M. Wang, J. J. Chen, I. A. Pikuleva, N. Mast, "Quantification of Histone Deacetylase Isoforms in Human Frontal Cortex, Human Retina, and Mouse Brain" *PLoS One*, Vol. 10, No. 5, (11-May-2015) (PubID: 916427)
- S. Muramoto, T. P. Forbes, A. C. van Asten, J. G. Gillen, "A Novel Test Sample for the Quantification of Illicit Drugs in Fingerprints using Imaging Mass Spectrometry" *Analytical Chemistry*, (27-Apr-2015) (PubID: 917378)
- Y. He, K. von Lampe, L. J. Wood, M. Kurti, "Investigation of lead and cadmium in counterfeit cigarettes seized in the United States" *Forensic Science International*, pp. 40-45, (08-Apr-2015) (PubID: 916111)
- D. A. Long, S. S. Wojtewicz, C. E. Miller, J. T. Hodges, "Frequency-agile, rapid scanning cavity ring-down spectroscopy (FARS-CRDS) measurements of the (30012)₂(00001) near-infrared carbon dioxide band" *Journal of Quantitative Spectroscopy and Radiative Transfer*, Vol. 161, pp. 35-40, (03-Apr-2015) (PubID: 917632)
- D. C. Ripple, L. Narhi, N. Afonina, S. Singh, A. Herre, P. Garidel, A. Koulov, V. Corvari, T. Spitznagel, P. Mangiagalli, I. Cecchini, K. Wuchner, T. Lubiniecki, H.C. Mahler, R. Schmidt, A. Polozova, P. Cash, A. Weiskopf, D. Nesta, M. Rossi, R. Simler, "Sub-visible (2 μ m to 100 μ m) particle analysis during biotherapeutic drug product development: Part 1, considerations and strategy" *Journal of Pharmaceutical Sciences*, Vol. 104, No. 6, pp. 1899-1908, (01-Apr-2015) (PubID: 913845)
- E. J. Petersen, "Measurement science challenges that complicate the assessment of the potential ecotoxicological risks of carbon nanomaterials" *Environmental Toxicology and Chemistry*, (01-Apr-2015) (PubID: 916487)
- P. Salipante, S. D. Hudson, "Model colloid system for interfacial sorption kinetics" *Langmuir*, Vol. 31, No. 11, pp. 3368-3376, (24-Mar-2015) (PubID: 917257)
- D. J. Audus, A. M. Hassan, E. J. Garboczi, J. F. Douglas, "Interplay of particle shape and suspension properties: a study of cube-like particles" *Soft Matter*, (20-Mar-2015) (PubID: 917500)
- R. A. Perkins, M. L. Huber, M. J. Assael, E. K. Mihailidou, S. K. Mylona, E. J. Sykioti, "Reference correlations for the viscosity and thermal conductivity of fluids over extended range of conditions: n-hexane in the vapor, liquid, and supercritical regions" *Pure and Applied Chemistry*, Vol. 87, No. 3, pp. 321-337, (11-Mar-2015) (PubID: 914943)
- N. D. Olson, J. M. Zook, S. P. Lund, F. Rojas-Cornejo, J. Huggett, J. B. Morrow, "International Interlaboratory Study Comparing Single Organism 16S rRNA Sequencing Data: Going Beyond Consensus Sequence Comparisons" *PLoS One*, (05-Mar-2015) (PubID: 915125)
- M. M. Schantz, R. S. Pugh, S. S. Vander-Pol, S. A. Wise, "Long-Term Stability and Temporal Trends of Organic Contaminants in four Collections of Mussel Tissue Frozen Standard Reference Materials" *Analytical and Bioanalytical Chemistry*, Vol. 407, pp. 3253-3258, (25-Feb-2015) (PubID: 916644)
- N. A. Schneck, M. S. Lowenthal, K. W. Phinney, S.B. Lee, "Current Trends in Magnetic Particle Enrichment for Mass Spectrometry-Based Analysis of Cardiovascular Protein Biomarkers" *Nanomedicine: nanotechnology, biology, and medicine*, Vol. 10, No. 3, pp. 433-446, (18-Feb-2015) (PubID: 915913)
- B. D. Ravel, W. Klysubun, C. Hauzenberger, P. Klysubun, Y. Huang, W. Wongtepa, P. Sombunchoo, "Understanding the blue color in antique mosaic mirrored glass from the Temple of the Emerald Buddha, Thailand" *X-Ray Spectrometry*, (04-Feb-2015) (PubID: 917140)
- N. Nadermann, E. P. Chan, C. M. Stafford, "Characterizing water transport in ultrathin desalination membranes using Quartz Crystal Microbalance with Dissipation" *ACS Applied Materials and Interfaces*, Vol. 7, No. 6, pp. 3492-3502, (19-Jan-2015) (PubID: 917221)

Full text versions of many papers and a full list of MML publications can be accessed through the NIST Publications Database at www.nist.gov/publication-portal.cfm

To learn more, contact:
Material Measurement Laboratory
100 Bureau Drive, M/S 8300
Gaithersburg, MD 20899-8300
Tel: 301-975-8300
Fax: 301-975-3845
mmlinfo@nist.gov
or visit <http://www.nist.gov/mml>

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