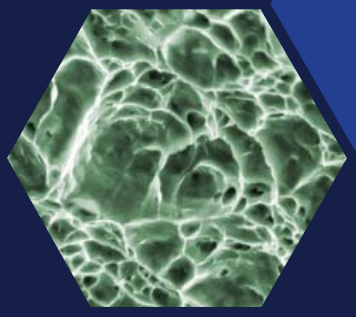
NIST | Material Measurement Laboratory Strategic Plan

2015



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

OUR VISION

Building the foundation for tomorrow's innovation in the Biological, Chemical and Materials Sciences.

OUR MISSION

To promote U.S. innovation and industrial competitiveness in the biological, chemical and materials sciences and technologies by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life.

Nearly every aspect of modern life relies on measurements:

NIST's Material Measurement Laboratory is the national reference laboratory for measurements in the chemical, biological and material sciences. MML provides basic science and practical tools for better, reliable measurements of complex chemical species, advanced materials, and biological systems. MML research produces new, sophisticated measurements of matter, as well as reference materials, reference data, and other practical tools that support a wide range of enterprises important to our nation, including healthcare, manufacturing, energy, infrastructure, and the environment.

OUR PLAN

This 5-year plan describes MML's priorities for establishing new measurement science and services to address emerging national needs, the operational and organizational innovations necessary to achieve our mission, and the means to sustain the wide range of technical efforts in MML that are key to our nation's economic success and quality of life.

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Continuously develop and provide the world-class measurement science expertise and capabilities needed to support economically critical U.S. enterprises in biology, chemistry and materials science and to underpin related global standards.

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GOAL 1 | MEASUREMENT SCIENCE EXCELLENCE

Biological Sciences Strategy 1: Complex Biotherapeutics

Develop measurement science, standards, and tools to support the quantitative definition of complex biologic therapeutics and correlation of their structural differences with clinical outcomes.

An overarching problem confronting the development, manufacturing, and regulatory approval of complex biotechnology medicines (e.g., protein, cell, gene, and nucleic acid therapies) is that these products cannot be adequately defined by measurement. This measurement gap leads to uncertainty in determining the consistency of products from different manufacturing batches or processes, and assessing the similarity of originator products with their biosimilar counterparts. MML will develop measurement science, standards, and tools to support the qualification of methods, assays, and instruments used to ascertain critical quality attributes of the product. MML will also develop bioinformatic tools for integrating analytical, biophysical, structure and bioassay data of these products to better enable prediction of their clinical performance.

To implement this strategy, MML will develop:

- Improved physico/chemical analytical and bioassay methods to better define product quality attributes of complex biologic therapeutics (cell therapies, proteins, vaccines, nucleic acids).
- Globally accepted reference standards to qualify and validate assays/methods/instruments used for characterization, release, or stability testing of biotechnological/biological products.
- A robust, open access bioinformatics toolbox for integrating the analytical, biophysical, structure, and bioassay data of a biologic into a structural map able to predict relevant clinical outcomes.
- A repository of NIST biologic reference materials to serve as a material resource for refining an analytical, biophysical, and bioassay characterization toolbox.
- Partnerships with key stakeholders including the biopharmaceutical industry, FDA, and other biotechnology-related organizations by convening workshops and roundtables to assess emerging trends and measurement needs, inform stakeholders of NIST capabilities, and leverage critical expertise not present at NIST.

Biological Sciences Strategy 2: Engineering Biology

Develop the measurements and models for engineering biology to map the fundamental principles that drive the development of the next generation of bio-based products.

Rapid advances in the ability to genetically modify biological organisms have created a new engineering discipline, termed 'synthetic biology.' This approach seeks to harness the power of living matter for a variety of manufacturing applications including advanced therapeutics, sustainable fuels, feedstocks, and advanced materials. Designing organisms for specific functions is currently done through trial-and-error, which is costly and inefficient. A more fundamental understanding of cellular control mechanisms will enable greater predictability of genetic modifications, but will also require precise and relevant data, based on sound measurement strategies. Synthetic biology itself can provide tools for designing and testing putative regulatory systems in cells. Applying high quality measurements to strategically designed systems will allow the development of mathematical models for analyzing response functions and extrapolating predicted responses. MML will establish the pipeline to connect tools for measuring, testing and controlling the interactions of synthesized biological systems with predictive testable models in a context of worldwide collaboration. The principles arising from the theoretical pipeline will drive understanding of the fundamental regulatory systems of biological organisms and will advance the field of synthetic biology.

To implement this strategy, MML will develop:

- Technical capabilities needed to achieve high-accuracy measurements (genomic, proteomic, metabolomic) on single cells, or small cell populations, and methodologies for determining uncertainties associated with these measurements.
- Test systems that integrate systematic genetic manipulation, precision measurements and predictive models.
- Data-sharing infrastructure to allow collaboration with academic and industrial partners.
- Collaborations with other federal agencies, academia, industry, and other partners, through workshops and scientific meetings, to leverage synthetic and systems biology communities in crowdsourced solutions to challenges.

Biological Sciences Strategy 3: Microbial Metrology

Develop measurement infrastructure for microbial measurements in health and environmental applications.

Over the past decade, researchers have renewed interest in microbiology, and in understanding the critical role microbes play in agriculture, manufacturing, food-safety, forensics, bioterrorism, energy, the environment, and medical therapies. This growing interest in microbial science is largely attributable to 1) recent understanding that complex microbial communities (microbiomes) are everywhere and play an important role in human health and the environment; 2) the spread of antibiotic resistance "superbugs" that have become a world health crisis and pose serious risks to modern medicine by thwarting our ability to treat common bacterial infections; 3) innovative diagnostic technologies for rapid and reliable detection and identification of pathogens in the clinic or in the environment. Yet the complexity of typical microbiomes is vast, and the measurement infrastructure urgently needed to support microbial measurements is daunting. Given these challenges, MML can play a vital role in advancing microbial metrology. Developing a robust infrastructure requires basic research as knowledge in the field develops, as well as new standards, methods, informatics approaches, and data that are yet to be established.

To implement this strategy, MML will develop:

- Quantitative tools, reference materials, and data for microbiome measurements.
- Bioinformatics capabilities needed to validate metagenomics data for microbial measurements in complex samples.
- A robust research program that includes work in antimicrobial resistance, tools for assessing biofilm organization, and rapid and sensitive pathogen detection.

Biological Sciences Strategy 4: Precision Medicine

Develop measurement science and standards to ensure confidence in clinical decision-making, and ultimately enable adoption of precision medicine.

The power of affordable and efficient 'next-gen' genomic sequencing and measurements of other biomarkers to aid personalized therapeutic treatment for individuals is rapidly leading to a revolution in health care. The successful transition of individualized therapies from the lab to the clinic, however, requires the development of a metrology infrastructure to assure the quality and reproducibility of diagnostic measurements. MML will develop measurement science, standards, reference data, and tools to assure the quality of genomic-, proteomic-, metabolomic-, and epigenomic-based diagnostics used in precision medicine therapies and clinical decision making.

To implement this strategy, MML will:

- Establish state-of-the-art whole genome sequencing and full analytical capabilities in metabolomics, proteomics, and gene expression analysis.
- Develop nucleic acid, protein, and other biomolecular reference materials to calibrate and assure the quality of clinical measurements.
- Engage other agencies, biopharma industry, academia, and clinician groups to determine emerging measurement needs and best practices for technology transfer of personalized biotherapeutics (protein biologics and cell therapies), through NIST-led workshops, participation in industry-led road-mapping exercises, and CRADAs with industry groups as appropriate to ensure access to clinically-relevant assays and samples needed.
- Establish a bioinformatics platform to integrate analytical data for predictive models, and to allow open access for all stakeholders.

Biological Sciences Strategy 5: Reproducibility of Biomedical Research

Establish NIST as a leader in biomedical measurement assurance to enable reproducibility of biomedical research results.

Many of the innovations in health care are founded upon data derived from living organisms. However, measurements of living systems are often not as straightforward as measurements of physical and chemical systems. Biological systems are complex and often poorly defined, and biological responses can be the aggregate result of an array of molecular events. These measurements are even more challenging because many biological responses are not discrete, but probabilistic in nature. These challenges often discourage researchers from approaching experimental design with robust and quantitative data outcomes in mind. While it is perhaps unsurprising then that many published findings have proven to be irreproducible outside of the original investigator's hands, it is imperative that the development of new therapeutic interventions be based on meaningful and reproducible data. NIST is a world-renowned expert in measurement sciences for the physical sciences, yet our profile in the biological sciences is still emerging. To maximize NIST's impact on the critical economic sector driven by biomedical research and fulfill our mission to 'promote U.S. innovation and industrial competitiveness' in applications of this research, NIST must enhance its reputation as a leader in measurement assurance for biomedical research.

To implement this strategy, MML will:

- Improve MML capabilities in innovative bioanalytical measurement technologies in prioritized cells systems research areas to develop, with the stakeholder community, foundational measurement protocols, reference materials, and data to ensure that NIST is an authoritative resource for these technologies.
- Raise NIST's profile with stakeholders in academia, other agencies, standards organizations, and science publishers through workshops and other outreach opportunities communicating the economic cost of failed biomedical studies due to invalid research design and execution, and frame NIST mission-space for this issue.
- Partner strategically with academia, standards-based organizations and consortia to promote training and educational opportunities for applying principals of biological metrology to biomedical research.

Chemical Sciences Strategy 1: Advanced Chemical Catalysis

Develop advanced measurement science, theory, and modeling to characterize and assess the factors governing the complex behavior inherent to novel chemical catalysis processes.

In a series of roadmaps and technical reports, American industry and other government agencies have identified the increasing need for a measurement science infrastructure based on the effective integration of advanced measurements, data, and modeling to understand complex catalytic processes. In particular, industrial partners have identified the need to develop a wide range of reference materials that could be characterized under sets of specifically controlled conditions to build more accurate and reliable simulation tools. These tools could be used by industry to accelerate the design and manufacturing processes of novel catalysts. This development would constitute a quantum leap in the current approach used by the scientific community, where currently models are empirically built and fine-tuned based on disparate sets of data produced in-house or available in the literature. By addressing these challenges and building the required measurement science infrastructure, NIST will position itself as the nation's "center of gravity," able to effectively translate fundamental measurement science and standards to improve the efficiency and cost effectiveness of the development of novel catalysts by our industrial stakeholders while at the same time minimizing the environmental impact of these processes.

To implement this strategy, MML will develop:

- Expertise in complexity theory, data science, and computational science.
- Novel measurement methodologies to provide accurate data that can be used to generate reliable models that are able to describe complex behavior in catalytic processes.
- Expertise in the synthesis of chemical and biological materials.

Chemical Sciences Strategy 2: Air Metrology for Our Changing Atmosphere

Develop the metrology for air quality needed to address evolving industries, new understandings of adverse health effects, changing energy sources, and the effects of climate change that face our nation.

Current issues such as climate change, changing energy sources, and new manufacturing practices continue to challenge our ability to measure, model, and manage air quality. To understand the impact of emissions, it is critical to have the capabilities to 1) identify and quantify the composition of emissions; 2) identify emission sources; and 3) understand how emissions evolve in the atmosphere through chemical and physical processes. Furthermore, the complex nature of the atmosphere coupled with processes that occur on multiple scales (local, regional, and global) and under different phases (gases, liquids, solids, and heterogeneous systems) present additional measurement and modeling challenges. With expertise in areas such as analytical chemistry, chemical kinetics, optical spectroscopy, and microanalysis combined with extensive customer interactions through a well-established standards program and relationships with other agencies, such as NASA, NOAA, and EPA, NIST is well-poised to address key questions and develop quality-assured measurements and data needed to provide a sound scientific foundation for evolving air quality policies and regulations.

To implement this strategy, MML will develop:

- Analytical capabilities in particulate measurements, isotopic analysis, and kinetics of heterogeneous systems.
- Next-generation data classification systems for anthropogenic and biogenic emissions.
- Scientific understanding, data, and reference standards to support measurements of particulates.

Chemical Sciences Strategy 3: Chemical Data Science and Informatics

Establish a chemical data science and informatics program to support the development of reliable and quantitative predictive modeling needed to advance a wide range of chemistry-related science and industrial enterprises.

The chemical science community is in need of reliable modeling tools that integrate measurements and quality data to advance both knowledge and technology. For example, in the biochemistry community the integration of data originating from different measurement techniques (NMR, MS, UV, etc.) as applied to different 'omics' (proteomics, metabolomics, and lipidomics) has been recognized as one of the most important challenges to achieving predictive strategies for healthcare. Similarly, a wide range of chemical science enterprises, including the design of advanced catalysis processes, complex chemical manufacturing routes, and the environmental sciences, would benefit from better data integration. By developing reliable modeling tools that integrate measurements and data, MML will address these ever-increasing needs in industry and the rest of the scientific community, thereby enabling researchers to design and interpret experiments targeted at the elucidation of complex chemical processes.

To implement this strategy, MML will develop:

- A team of chemometricians, data scientists, and software development experts that complement the extensive chemical measurement expertise in MML.
- Technical efforts that integrate new capabilities in chemical data and informatics with our measurement capabilities to create new tools for predictive chemical science, including new SRM, and SRD modes, and validated models that advance predictive modeling for the environmental sciences, catalysis, and chemical manufacturing.

Chemical Sciences Strategy 4: Chemical Manufacturing

Develop the measurements needed to monitor and optimize chemical processes for the manufacture of the advanced specialty chemicals and functional materials that will keep our nation at the forefront of technological innovation.

The manufacture of new specialty chemicals and functional materials, with applications as varied as sensing, catalysis, and advanced formulations, involve exotic reactants with complicated reaction pathways, reaction intermediates, and chemical kinetics that are poorly understood and rarely quantified. Even basic physical and chemical properties needed for process control, such as the temperature dependence of vapor pressure, are often not known for these advanced products. Traditionally, chemical engineers have been able to fashion hard-won empirical approaches to address highly specific manufacturing routes. However, these approaches are largely not guided by quantitative measures and validated models that could optimize product yield and reduce the use of expensive and often toxic reagents in a more comprehensive manner. A better approach is to use sound and reliable physicochemical properties to optimize the manufacturing process using models, validated through measurement of key reaction steps and rates.

To implement this strategy, MML will develop:

- Innovative model chemical reactors and fabrication tools that replicate industrial process, but that are equipped with monitoring instruments and sensors that can quantitatively assess key process factors.
- Computational tools and experimentally-validated models to simulate chemical processes used in manufacturing advanced specialty chemicals and functional materials.

Chemical Sciences Strategy 5: Comprehensive Measures of Water Quality

Develop advanced, broad spectrum organic, inorganic, and biological measurement capabilities and standards for assessing the quality of water, to ensure that the U.S. has the tools needed to effectively manage its water resources now and in the future.

The effective management of our water resources now and in the future is critical to ensure sustainability for manufacturing, energy, food production, and health. Presently, our freshwater supplies are being threatened by well-known and emerging contaminants, climate change, and overuse, placing the nation at risk for increased water shortages and negative health impacts. At the same time, there is a need to utilize less pristine, alternative water sources including recycled wastewater, saline water, storm water run-off, rainwater, and industrial by-process water in our future water management plans. To ensure proper resource management, it is critical to determine what chemicals and microbiological organisms are present in a wide range of traditional and alternative water resources to determine 'fit-for-purpose' water usage, particularly for applications that do not require potable-quality water (e.g. agriculture and certain industries).

To implement this strategy, MML will develop:

- Broad spectrum, comprehensive measurement capabilities that are applicable to all water supplies and are robust to samples with widely-variable compositions, supporting the water measurement and monitoring needs of other government agencies and industry.
- Expertise in multivariate analysis for both comprehensive chemical and biological datasets and for seamless data integration.
- Measurement and data analysis capabilities for sensor validation.

Materials Sciences Strategy 1: Additive Manufacturing

Develop the material measurement infrastructure that will enable additive approaches to production to prosper and revitalize manufacturing in the U.S.

Additive manufacturing promises to revolutionize not only how objects are designed and manufactured, but also how materials are specified, processed, characterized, and used. Additive manufacturing includes all types of technologies for the creation of three-dimensional objects from digital data by incrementally adding material. The properties, performance, and reliability of the final products made by these processes are determined by the unique processing or joining technology used to bond these increments and the microstructures that result. MML can play a vital role in enabling the growth and prosperity of this emerging industry by developing an infrastructure of material measurements, standards, data, and models that enable a more fundamental understanding of these processes and the materials and processing variables that influence final product quality.

To implement this strategy, MML will develop:

- Measures of precursor characteristics that relate to performance in additive processes and the properties of final products.
- Measurement methods, data, and models that can be used to guide improvements in consolidation including greater control of microstructures, properties, residual stresses, and distortion.
- Measurement techniques for characterizing the properties, performance, and reliability of the materials and microstructures produced by additive technologies.
- Measurement tools, data, and models for detecting and understanding the influence of additive processing defects on product performance and reliability.

Materials Sciences Strategy 2: Dynamic Measurements for Materials Manufacturing

Expand measurement capabilities that provide a detailed view of materials in dynamic environments that are critical to key technological areas and advanced manufacturing routes.

While being processed, manufactured into products, or operating in products, materials are fundamentally non-equilibrium in nature. During processing, manufacture, and use, rapidly changing state variables (e.g., temperature, electrostatic potential, chemical gradients) induce transitory responses in fundamental materials characteristics, such as composition, morphology and strain, and charge densities. Industry needs tools to provide insight into how their processes control and create exploitable transitory phenomenon of materials in their products. These challenges require better data, information, and the science of materials structure, properties, and behavior under dynamic manufacturing and operational (processing) conditions. This means increasingly sophisticated in-line measurement methods and data on materials response under non-equilibrium or dynamic conditions relevant to the processing environment.

To implement this strategy, MML will:

- Develop capabilities to measure functional materials *in operando* with high spatial and temporal resolution.
- Develop new measurement capabilities of materials during processing and under operation.
- Demonstrate connections between NIST measurements in the laboratory with manufacturing processes.
- Focus on and partner with the National Network for Manufacturing Innovation programs.

Materials Sciences Strategy 3: A Foundry for Functional Materials Measurement

Invest in capabilities to synthesize materials with the composition, structure, and properties needed to enable leading edge materials measurement science.

The substantial national investment in advanced materials discovery and development is continually producing innovative materials with the potential to revolutionize a vast array of technologies that could expand economic growth in the U.S. Recent examples include 2D materials for electronics with unprecedented performance, soft materials and polymers that are responsive to their environment, and multi-component functional materials that can harvest energy. For these new discoveries, persistent gaps exist between the initial material creation, the establishment of high-quality and consistent robust synthesis methods, and the establishment of a consensus measurement system. To address these gaps, MML needs the capabilities to produce a range of materials to enable the highest quality measurements of their intrinsic properties and performance.

To implement this strategy, MML will develop:

- New synthesis facilities needed to produce the highly controlled materials or materials libraries needed to provide reliable measurement of promising materials.
- A sustainable operational model to enable both the capability to make new materials and provide support for a broad range of programs.
- Capabilities to fabricate materials and devices into functional devices or within operating environments.

Materials Sciences Strategy 4: Infrastructure Renewal

Develop fundamental measurements of materials degradation in service environments to predict performance, estimate service life, and accelerate remediation of critical infrastructure.

The U.S. maintains an extensive network of civil infrastructure to ensure public health, safety, security, and commerce. Deterioration due to aging, chemical attack, and mechanical fatigue places these structures at risk for failures, and will eventually cost the U.S. hundreds of billions of dollars. A significant barrier to the consideration of innovative alternatives is the lack of fundamental materials models that enable the correlation of service history (including loading and environmental conditions) to reduction in structural capacity in infrastructure components and systems. Such models would guide the development of new infrastructure materials resulting in more effective, lower cost solutions. Successful development and deployment of these models requires an understanding of the fundamental mechanisms of chemically-assisted, stress-induced degradation found in service. In addition, standardized tests and tools are required to quantify the reduction in performance of exposed components. Databases and supporting informatics tools will adopt and build upon those developed under the NIST Materials Genome Initiative (MGI) program.

To implement this strategy, MML will develop:

- Measurement methods and data to identify fundamental degradation mechanisms in the relevant infrastructural materials and exposure (chemical and mechanical) environments.
- Measurement science for determining the time-dependent change in the mechanical properties of materials as a function of service history (loading, environment).
- Databases of materials, mechanisms, and data for use in performance measurement prediction, through adoption of tools developed under the Materials Genome Initiative.

Materials Sciences Strategy 5: The Materials Genome Initiative

Realize the full potential of the Materials Genome Initiative (MGI) through the development and delivery of a National Materials Innovation Infrastructure and by broadening the range of technology areas that can benefit from MGI-related tools.

Today, the discovery, design, development, and deployment of new materials for innovative products is a time-consuming and laborious process, as much a craft practiced by skilled artisans as a science. The task of designing a new material is extremely complex, involving many factors that must be balanced. A powerful new tool for materials discovery and optimization has begun to emerge: computational materials by design. To this end, the goal of the National Material Genome Initiative (MGI) is to establish an innovation infrastructure that integrates, tests, and disseminates data, computational models, and experiment for different technology areas and materials classes. In contract to heuristic approaches, NIST contributions to the MGI will yield quantitative, predictive computational capabilities founded on both data-driven and physics-based material models, leading to shorter development times, materials of improved performance, and better products – with a focus on the reliability of these computational approaches. To achieve these aims, MML will establish and leverage validated experimental data streams, improved methods for integrating experimental data and models, as well as new routes for determining uncertainties in predictive models and simulations.

To implement this strategy, MML will develop:

- Materials data and model exchange protocols essential for a broad range of materials researchers to better access and use the universe of information and predictive capabilities that could accelerate their discovery efforts.
- Widely applicable tools and protocols that ensure, or at least transparently gauge, the quality of materials data and models, including uncertainty.
- New methods, metrologies, and capabilities necessary for accelerating development of critical classes of advanced materials, including high-temperature alloys, polymer materials and composites, and biomaterials.

GOAL 2 | MEASUREMENT SERVICE EXCELLENCE

Broaden access to and impact of NIST reference products and standards to accelerate innovation, support the creation of new industries, and enhance global commerce and trade.

Strategy 1

Examine and update the goals, vision, and implementation of the NIST Standard Reference Data Program to drive improvement of the quality of available NIST data products, the utility of such data for stakeholders, and its sustainable stewardship.

Strategy 2

Invigorate the NIST SRM program and enable dedication of resources to emerging measurement problems by implementing new, more efficient, certification modes for renewal of legacy SRMs.

Strategy 3

Develop a new class of research-grade materials that have a significantly shorter development time compared to SRMs and RMs so that NIST can provide measurement tools that meet industry's rapidly changing needs on a timely basis.

GOAL 2 | MEASUREMENT SERVICE EXCELLENCE

Strategy 1: Modernization of Standard Reference Data

Examine and update the goals, vision, and implementation of the NIST Standard Reference Data Program to drive improvement of the quality of available NIST data products, the utility of such data for stakeholders, and its sustainable stewardship.

NIST has produced and published Standard Reference Data (SRD) for nearly fifty years. The Mass Spectral Library with Search Program (Mass Spec), Reference Fluid Thermodynamic and Transport Properties (REFPROP), and Inorganic Crystal Structure Database (ICSD) are examples of three highly visible and active SRD data products. MML has responsibility for SRD throughout NIST, including data products maintained by MML, as well as by NIST's Physical Measurement and Information Technology Laboratories (PML, ITL), many of which have not changed in ten years or more. To continue to meet the needs of our customers for curated materials property data, MML will initiate a modernization effort to examine the SRD program. Through a series of collaborations with internal stakeholders, MML will evaluate the SRD infrastructure to improve discoverability and ease of use, while deploying new technologies such as application programming interfaces. Additionally MML will examine the definition of SRD, define SRD quality, and align the SRD program with NIST's Open Data efforts. The success of this strategy depends on the ability to openly examine the Standard Reference Data program, understanding existing procedures, and collecting and communicating impact metrics of SRD data products. The success is further dependent on defining the relationship between SRD, SRMD, and other reference data programs in MML and at NIST.

To implement this strategy, MML will:

- Establish an SRD program review committee and SRD advisory team to suggest improvements to the SRD program by determining the impact of SRD, prioritizing products in need of updates, and addressing SRD quality.
- Improve public access to SRD by updating the SRD homepage, enhancing the data gateway, and creating a common look and feel across NIST web products.
- Implement applications programming interfaces by leveraging Socrata software and positioning SRD to benefit from the NIST data infrastructure fund.
- Review the economic model for SRD development and maintenance, investigate the feasibility of an improved funding model for SRD to enhance existing products and facilitate new SRD initiatives, and issue a request for proposals for new SRD applications.

GOAL 2 | MEASUREMENT SERVICE EXCELLENCE

Strategy 2: New Certification Modes for Reference Materials

Invigorate the NIST SRM program and enable dedication of resources to emerging measurement problems by implementing new, more efficient, certification modes for renewal of legacy SRMs.

Once particularly impactful SRMs are produced and adopted for use, customers become dependent on them as integral parts of traceability schemes for measurement systems. When no alternative approach to benchmarking measurement accuracy is available, customers depend on NIST to continue to reliably produce such SRMs. Many times the renewal of popular SRMs provides no new measurement challenges for NIST scientists, and the renewal process takes away from valuable R&D on cutting edge topics. A solution to this challenge is to examine a new certification mode for renewal SRMs that relies on measurement protocols carefully designed by NIST, but that are executed by trusted NIST partners. NIST would be responsible for the detailed experiment design including the use of blind control materials. NIST would choose measurement partners who would actually perform the measurements according to the protocols. NIST would then evaluate the data, including control results and produce the certified/reference values and uncertainties. Effective implementation of these approaches will be marked at first by the adoption of the scheme in the annual project proposal stage and later by the successful renewal of critical SRMs using measurement data generated by collaborators.

To implement this strategy, MML will:

- Employ a NIST Traceable Reference Material-like model for highly repetitive batch production.
- Implement a certification mode that involves a NIST-designed protocol and controls, with outside collaborator analysis data.
- Increase technician staffing, when appropriate, to amplify the impact of PhD staff involved in SRM development and renewal.
- Implement prioritization processes to ensure that only high impact/critical SRMs are renewed or undertaken by NIST.

Strategy 3: A New Class of Reference Materials

Develop a new class of research-grade materials that have a significantly shorter development time compared to SRMs and RMs so that NIST can provide measurement tools that meet industry's rapidly changing needs on a timely basis.

According to the ISO/REMCO Committee, reference materials must have prescribed homogeneity and stability of a measurand to be feasible. Once the feasibility testing to determine material homogeneity and stability has been completed, NIST Standard Reference Materials (SRMs) and Reference Materials (RMs) require, on average, an additional three years to produce. However, there are many cases where industry stakeholders need a material with just the basic features of a reference material to benchmark measurements in rapidly emerging fields. Oftentimes, such a material is all that is required for stakeholders to begin sorting out measurement comparability problems in the early stages of new technology areas. NIST can better serve such challenges by developing a new class of reference or research material standards, combined with a plan to progress from feasibility to production in one to two years or less.

To implement this strategy, MML will develop:

- Research materials as a class of reference materials with prescribed homogeneity and stability.
- A data submission process and repository so that outside stakeholders can continue to contribute to the characterization of the material.
- A process and knowledge base to engage stakeholders and identify 'trusted' laboratories for characterization and value-assignment.
- A business model that facilitates distribution to the public at low cost.
- A "graduation" approach for promoting quality research materials to SRM status as needed by the community.

GOAL 3 | DATA SCIENCE AND DATA MANAGEMENT CAPABILITIES

Build the infrastructure for next-generation data science tools and the management of complex data sets needed to support scientific innovation and advance open data concepts in the biological, chemical and materials sciences.

Strategy 1

Establish the Office of Data and Informatics, and position it as a broker to provide solutions for data and informatics problem analysis for both MML and its customers.

Strategy 2

Build the data informatics and analytics capabilities and establish related best practices needed for MML to address the climate of increasingly complex and data driven measurement research challenges.

Strategy 3

Establish NIST as the leading organization for convening broad discussions and charting a course towards increasing the availability of quality data related to biology, chemistry, and materials science.

Strategy 4

Address data management challenges that currently hamper external partnerships in MML.

GOAL 3 | DATA SCIENCE AND DATA MANAGEMENT CAPABILITIES

Strategy 1: A Data and Informatics Solutions Broker

Establish the Office of Data and Informatics, and position it as a broker to provide solutions for data and informatics problem analysis for both MML and its customers.

The MML Office of Data and Informatics (ODI) was established in 2014 to serve four major functions: managing the Standard Reference Data collection, improving research data management infrastructure and functions, establishing communication and collaboration with the national and international community of data organizations and practitioners, and providing expertise and guidance related to informatics and analytics capabilities and tools. As a solutions broker, ODI will reach out to MML staff to glean key needs, guide improvements to data management systems and services, and where resources allow pilot and deploy data management solutions. Once fully developed in this capacity, the ODI will serve as a "storefront" of data management related services and tools.

To implement this strategy, MML will:

- Establish and deploy in-reach mechanisms for determining and prioritizing key data challenges faced by MML and NIST staff.
- Build expertise in data management systems relevant to the physical sciences and geared towards addressing priority MML data challenges.
- Develop and deploy excellent science data management facilities, aimed at improving accessibility and usability of MML data products and assuring compliance with federal Open Data policies and practices.

GOAL 3 | DATA SCIENCE AND DATA MANAGEMENT CAPABILITIES

Strategy 2: Informatics and Analytics Capabilities

Build the data informatics and analytics capabilities and establish related best practices needed for MML to address the climate of increasingly complex and data driven measurement research challenges.

As research datasets become both larger and more complex, analysis and knowledge extraction tools must be developed and adapted to deal with scale, heterogeneity, and traceability. At one extreme, researchers require fundamental advances in research tools - developed in collaboration with computer scientists, statisticians, and big data analytics specialists both within and outside of NIST. Many data-centric analysis problems have well-established solutions, though best practices may not be known to MML bench scientists. Through communication and collaboration MML research will be improved, with robust uncertainty analysis, trend assessment, and pattern recognition in complex parameter space.

To implement this strategy, MML will:

- Establish informatics expertise in MML and liaise with the broader community of NIST and external informatics experts in order to advise and support staff who face data-driven research challenges.
- Create a software library and computational infrastructure to support the use of advanced informatics and analysis methods for NIST staff.

GOAL 3 | DATA SCIENCE AND DATA MANAGEMENT CAPABILITIES

Strategy 3: Leadership in Sharing High Quality Scientific Data

Establish NIST as the leading organization for convening broad discussions and charting the course towards increasing the availability of quality data related to biology, chemistry, and materials science.

As demonstrated by its already extensive data services, NIST and MML are a national and world resource for fundamental, well-characterized data in biology, chemistry, and materials science. As such, NIST and MML should provide easy and open access to its data products and services. MML-produced data should be disseminated more effectively, used and repurposed more widely, and cited. In addition, data associated with the development of our best measurement science and measurement capabilities should be disseminated whenever possible. To meet our own data sharing aims, and that of the broader community, as a national standards organization MML should provide leadership in building consensus around standards that promote data discovery, access, re-use, and reproducibility. Such efforts will enable broad and reliable data provision, data preservation, and curation activities that will permeate data management activities in bench science, simulation, and Standard Reference Data generation and stewardship. If successful, this effort will lead to more extensive citation of NIST/MML data products, the use of NIST/MML data in innovative and unanticipated applications, and recognition of NIST as an exemplar federal agency in data management practices.

To implement this strategy, MML will:

- Through a series of stakeholder workshops, promote discourse within NIST and more broadly in the research community to identify and foster best practices in data sharing and demonstrate their value to all levels of an organization.
- Enhance our ability to build best practices by developing strategic partnerships among institutions that are more experienced in large scale data sharing.
- Create an ODI fellow program to foster collaboration with knowledgeable individuals from identified institutions.

Strategy 4: New Data Management and Data Sharing Approaches

Address data management challenges that currently hamper external partnerships in MML.

Effective use of data with NIST/MML partners requires enumerating and identifying the data management challenges that we face together. We will strive for discoverability and interoperability with key partners, such as our Centers of Excellence, to advance data-enabled research and development. We will establish data sharing environments and tools that demonstrate the benefits of data-based collaboration.

To implement this strategy, MML will:

- Examine existing partnerships and identify current data management needs.
- Establish data management plans and practices that facilitate data sharing and re-use.

GOAL 4 | STRATEGIC PARTNERING

Actively engage with customers, partners, stakeholders, and collaborators to expand our scientific reach and heighten our customer focus.

Strategy 1

Broadly engender staff with the values of customer engagement and the best practices of outreach and partnership mechanisms they need to identify and effectively collaborate with strategic partners and stakeholders.

Strategy 2

Establish targeted partnerships to better leverage our resources, understand customer needs, and gain access to needed talent.

GOAL 4 | STRATEGIC PARTNERING

Strategy 1: A Culture of Outreach

Broadly engender staff with the values of customer engagement and the best practices of outreach and partnership mechanisms they need to identify and effectively collaborate with strategic partners and stakeholders.

A core value of MML is to develop technical programs that meet the needs of our stakeholder community, and this requires constant attention to outreach. While our track record in this regard is sound, deliberate training on customer engagement will ensure that every generation of MML staff can connect with relevant customers, determine when partnering is mutually and strategically valuable, identify the appropriate partnering mechanism, and formalize the partnership quickly and efficiently so that collaborative research can proceed. This strategy focuses on ensuring that MML staff can easily access the resources they need to guide them through the partnering process. Such resources include highlights and lessons learned from successful partnerships, step-by-step instructions for key activities (e.g., hosting a stakeholder meeting, developing a Material Transfer Agreement, or establishing a CRADA), and contacts that can provide direct assistance.

To implement this strategy, MML will:

- Host a series of internal workshops focused on strategic partnerships, showcasing success stories and including presentations and discussion with representatives from both MML and our stakeholder community.
- Create an internal website with best practices, links to appropriate resources, and brief "how-to" descriptions ranging from consortia models to best practices for web conferencing.

GOAL 4 | STRATEGIC PARTNERING

Strategy 2: Targeted Partnerships

Establish targeted partnerships to better leverage our resources, understand customer needs, and gain access to needed talent.

Partnerships with other agencies, industry, and universities can greatly enhance MML's success at all stages of program development and implementation. Effective partnering can help to ensure that MML research addresses the highest priority issues facing its customers and provide additional resources (e.g., people, skills, equipment, and funding) to carry out the necessary research. Targeting partnerships in key research areas can also accelerate the adoption of MML products, increase the impact of MML scientists, and enable MML to combine its expertise with complementary external skills to address broad multidisciplinary problems. This strategy seeks to assess areas in need of strategic partners, provide assistance in identifying and establishing such partners, and improve the mechanisms for cross-site communication.

To implement this strategy, MML will:

- Determine areas in which targeted partnerships will best serve MML strategic goals and key national needs.
- Deploy dedicated staff (e.g., MML Program Directors, NIST Emeriti, and AAAS Fellows) to assist in identifying and establishing key partners.
- Invest in improved VTC mechanisms, conference facilities, and web interfaces to achieve the communications necessary to maintain our focus on increasing partnerships in lieu of increasing travel.

GOAL 5 | ORGANIZATIONAL EXCELLENCE

Develop the leadership depth, breadth of technical capabilities and staff talents, and administrative expertise and processes needed to excel in our mission.

Strategy 1

Establish practices with a long term perspective for hiring, career development, and retention to support technical excellence within the organization.

Strategy 2

Develop a safety culture that integrates policies and procedures from NIST-wide safety programs into the daily research activities of all staff members, and that is resilient to management and organizational changes.

Strategy 3

Develop a program for acquiring and optimizing the utilization of high-value, unique resources and equipment critical to MML program areas in biology, chemistry and materials science.

Strategy 4

Continue to develop practices and tools to augment the efficiency and effectiveness of administrative functions, and reduce the administrative workload on technical staff.

Strategy 5

Build a sustained and purposeful leadership development program to broaden and deepen our pool of potential formal leaders, and to enrich the careers of our staff.

GOAL 5 | ORGANIZATIONAL EXCELLENCE

Strategy 1: Best-Fit Talent for Technical Excellence

Establish practices with a long term perspective for hiring, career development and retention to support technical excellence within the organization.

As MML programs evolve, so should our staff. Historically, MML scientific staff have tended to focus their careers in one discipline or programmatic area. In today's environment, programmatic needs are shifting due to new innovations, industry needs, and a changing regulatory landscape. MML will create an environment where our leaders and staff are encouraged to explore new opportunities to enable the advancement of MML programs. In addition, the hiring of new technical staff will be fine-tuned to meet our needs. We will assess the competences required for each position and hire staff best-suited for that role, to develop a nimble organization with highly engaged leaders and staff.

To implement this strategy, MML will:

- Deliberately and actively guide our staff's professional careers through targeted recognition and performance management programs, as well as career development driven by opportunities for autonomy, creative exploration, and elevated levels of service.
- Enhance the attractiveness of employment in MML by articulating the value of our service to the nation, and promoting our world-class mentor expertise and facilities, intellectual empowerment, and work-life balance.
- Increase the hiring of entry level technicians and engineers to amplify the efforts of MML PhD level staff, and to provide stewardship for shared facilities.
- Develop an MML-wide hiring plan for building the technical expertise required to meet our mission.

GOAL 5 | ORGANIZATIONAL EXCELLENCE

Strategy 2: An Integrated and Sustainable Safety Culture

Develop a safety culture that integrates policies and procedures from NIST-wide safety programs into the daily research activities of all staff members, and that is resilient to management and organizational changes.

NIST is a world-class scientific organization that utilizes instrumentation, equipment, biological specimens, chemicals, and radiological materials to achieve its measurement sciences mission. Understanding and mitigating the hazards associated with these items is critical to ensuring the safety of staff and property. Recently, NIST has rejuvenated its safety programs to ensure current regulations, policies and procedures are being followed and to ensure comprehensive coverage of all potentially hazardous activities, materials, and equipment within the organization. The critical next step toward promoting a safe working environment is to successfully and seamlessly integrate the NIST-wide safety programs into MML's day-to-day operations. Another important goal is to minimize the total number of hazardous materials located within our laboratories.

To implement this strategy, MML will:

- Actively engage with NIST safety professionals to ensure our safety measures are appropriate for the tasks being performed in each laboratory.
- Convene annual MML safety days and improved inspection procedures to identify and reduce hazards in our laboratories.
- Develop a sustainable process for actively managing biological, chemical, and radiological materials to minimize potential hazards and to prevent legacy items.

Strategy 3: Optimized Technical Capabilities

Develop a program for acquiring and optimizing the utilization of high-value, unique resources and equipment critical to MML program areas in biology, chemistry and materials science.

A critical factor for the success of MML programs is the sustainability of state-of-the-art technical capabilities. Because of the complex technical nature of MML scientific research, large equipment procurement and upkeep can present challenges to annual laboratory budgeting. The laboratory should formulate strategies to better manage our equipment needs, and develop mechanisms for meeting our technical needs across the lab.

To implement this strategy, MML will:

- Identify mechanisms to support MML-level equipment procurement, distinct from Division equipment funds.
- Complete an assessment of 1) the specialized skills required to maintain equipment and resources essential to cross-division MML Programs, 2) the types of equipment that fit a multi-division model, and 3) current Laboratory equipment that could be more effectively utilized if part of a multi-division equipment model.

Strategy 4: Streamlined Administrative Functions

Continue to develop practices and tools to augment the efficiency and effectiveness of administrative functions, and reduce the administrative workload on technical staff.

In today's federal environment, administrative functions have increased significantly and are time consuming for MML technical staff. MML has to strike the right balance for technical staff by taking ownership of these necessary administrative functions while allowing staff to perform their scientific functions. MML has taken steps in this direction, leading NIST in developing new systems and tools to facilitate interactions with NIST Management Resources organizations. Continuing these efforts, MML will work to develop an end-to-end system to streamline administrative functions, provide the ability for dynamic real-time financial planning, acquire efficient, timely, and compliant electronic approvals and purchases, and fulfill timely reporting information.

To implement this strategy, MML will:

- Conduct an analysis of the cost/impact of administrative processes on MML staff, in order to identify key areas where increased training, additional support staff, or other investments are needed to streamline administrative functions.
- Create a modern framework of opportunities for career advancement for administrative and support staff.
- Invest in applications and process improvements modeled on our past successes with NISTOrg and the MML Hazard Review Database.
- Develop a "one stop shop" for all administrative functions.

GOAL 5 | ORGANIZATIONAL EXCELLENCE

Strategy 5: Sustainable Leadership

Build a sustained and purposeful leadership development program to broaden and deepen our pool of potential formal leaders, and to enrich the careers of our staff.

A critical factor in ensuring long term success for MML is a viable leadership program that supplements the current NIST leadership programs. Key goals of leadership development are to promote leadership and to prepare current and aspiring leaders for the demands of today as well as the challenges of tomorrow. In the past, MML has had difficulty recruiting people into leadership positions, both formal (Group Leader/Division Chief) and informal (technical leaders). An enhanced leadership program will seek to increase recognition of leadership in the organization in ways that articulate 1) the value of leadership in MML, and 2) the value proposition of formal and informal leadership positions for staff. MML will focus on finding mid-career technical professionals looking for leadership opportunities, develop expected succession plans for Group Leader and Division Chief positions, and encourage broad participation in leadership workshops and training.

To implement this strategy, MML will:

- Assess the current state of leadership training and opportunities in MML and then design a training system to fill in the gaps.
- Create an MML mentorship program.
- Arrange for an external evaluation of MML's Leadership Program.

NIST | Material Measurement Laboratory Strategic Plan

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