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## An Assessment of the Material Measurement Laboratory at the National Institute of Standards and Technology: Fiscal Year 2020 (2021)

### DETAILS

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**AN ASSESSMENT OF THE  
MATERIAL MEASUREMENT LABORATORY AT THE  
NATIONAL INSTITUTE OF STANDARDS AND  
TECHNOLOGY**

**FISCAL YEAR 2020**

Panel on Review of the Material Measurement Laboratory at the  
National Institute of Standards and Technology

Laboratory Assessments Board

Division on Engineering and Physical Sciences

A Consensus Study Report of

*The National Academies of*  
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## Acknowledgment of Reviewers

This Consensus Study Report was reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise. The purpose of this independent review is to provide candid and critical comments that will assist the National Academies of Sciences, Engineering, and Medicine in making each published report as sound as possible and to ensure that it meets the institutional standards for quality, objectivity, evidence, and responsiveness to the study charge. The review comments and draft manuscript remain confidential to protect the integrity of the deliberative process.

We thank the following individuals for their review of this report:

Stuart Cooper, NAE,<sup>1</sup> The Ohio State University,  
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Newell Washburn, Carnegie Mellon University.

Although the reviewers listed above provided many constructive comments and suggestions, they were not asked to endorse the conclusions or recommendations of this report nor did they see the final draft before its release. The review of this report was overseen by David W. Johnson, Jr., NAE, Bell Laboratories, Lucent Technologies. He was responsible for making certain that an independent examination of this report was carried out in accordance with the standards of the National Academies and that all review comments were carefully considered. Responsibility for the final content rests entirely with the authoring committee and the National Academies.

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## Summary

In 2020, at the request of the Director of NIST, the National Academies of Sciences, Engineering, and Medicine formed the Panel on Review of the Material Measurement Laboratory of the National Institute of Standards and Technology (the “panel”), having earlier established the following statement of work:

The National Academies of Sciences, Engineering, and Medicine Panel on Review of the Material Measurement Laboratory at the National Institute of Standards and Technology will assess the scientific and technical work performed by the National Institute of Standards and Technology (NIST) Material Measurement Laboratory. The panel will review technical reports and technical program descriptions prepared by NIST staff and will visit the facilities of the NIST laboratory. The visit will include technical presentations by NIST staff, demonstrations of NIST projects, tours of NIST facilities, and discussions with NIST staff. The panel will deliberate findings, conclusions, and recommendations in a closed session panel meeting and will prepare a report summarizing its assessment of findings, conclusions, and recommendations.

The assessment shall be responsive to the charge from the NIST Director. The following are the criteria for the assessment:

1. The technical merit of the current laboratory program relative to current state-of-the-art programs worldwide;
2. The portfolio of scientific expertise as it supports the ability of the organization to achieve its stated objectives;
3. The adequacy of the laboratory budget, facilities, equipment, and human resources, as they affect the quality of the laboratory's technical programs; and
4. The effectiveness by which the laboratory disseminates its program outputs.

The Material Measurement Laboratory (MML) comprises six technical divisions and two offices. The two offices manage programs related to NIST standard reference materials (SRMs) and NIST data products or standard reference data (SRD). The technical divisions engage in research and development of the measurement science, standards, technology, and data required to support the nation’s need to design, develop, manufacture, and use materials. These divisions interact extensively with both industry and public institutions to advance the economy and provide tools for the creation of knowledge.

## GENERAL CONCLUSIONS

The study identified a number of themes across the MML divisions and offices regarding the high technical quality of the research, excellence of the scientific staff, strong customer outreach and scientific collaboration, and strong publication and dissemination activities. The recommendations in the following sections are grouped by division or office to provide actionable suggestions that address the unique needs of each; the two or three recommendations judged to be of greatest urgency for each division or office are included here in the Summary. Such recommendations address issues that could impact the mission of MML or NIST in the judgment of the panel; these can include, for example, issues that have been elevated by NIST stakeholders, other federal agencies, or Congress or identified through some other

mechanism. There are, in addition, several crosscutting themes that fall within the four items of the panel's statement of task that will be discussed first.

As regards technical adequacy, MML conducts research that is exceptional. It has formal arrangements with renowned institutions such as Brookhaven National Laboratory and, in the Institute for Bioscience and Biotechnology Research, two campuses of the University of Maryland system. The global reach and influence of MML is evident from the leadership roles the staff have taken in international standards development organizations. Further, nearly half the requests for SRM originate from outside the United States. From this, the panel infers that MML is competitive or ahead of the state-of-the-art worldwide in standards development and metrology. The panel's review shows that, as the portfolio of SRM expands into new areas such as biology, the MML will need to consider how to optimally allocate resources between maintaining legacy SRM versus re-purposing those resources toward SRM and SRD in new and emerging areas.

As regards the portfolio of scientific expertise, the resilience of MML's program to retirements or unforeseen departures could be improved. In some places, there needs to be more systematic succession planning to prevent gaps from occurring. Cross-training to provide backup coverage in case the primary cognizant scientist leaves is a further way to protect against disruption. In other instances, retraining to take on emerging issues requiring different disciplinary knowledge is lacking.

With respect to the adequacy of laboratory budget, facilities, equipment, and human resources, the research equipment utilized in the divisions supports or enables the delivery of MML's mission. The purchase, renewal, and maintenance of such equipment—including maintaining the buildings that house them—are effected through a set of business practices and attitudes. The purchasing power of the divisions is impacted first by a 50 percent tax on equipment. This disadvantages equipment purchases for purposes of budgeting as the trade-off versus funding an additional staff position or other expenditures becomes more acute. Further, the NIST working capital fund model for purchase of new equipment requires payback for any purchase from annual operating funds. MML also noted continuing challenges of aging and outdated building infrastructure and of "large" equipment needs and uses.

Complicating this is the ongoing challenge in finding resources for maintaining existing infrastructure (leaky roofs, HVAC [heating, ventilation and cooling] in need of repair, etc.). Although equipment and staff are appropriately prioritized over buildings, there have been instances where failures of the infrastructure compromised equipment and had an impact on mission delivery. The buildings on the main NIST campus may have exceeded their design life and are otherwise in need of repair. Finding resources to address this is difficult but critical to maintaining infrastructure that is consistent with, and will support operations of, exquisitely sensitive instruments and the brand for excellence that is associated with NIST worldwide. This includes modular laboratories that are flexible in use and can be relocated and/or reconfigured within a new room/building. It was apparent during the review meeting that some divisions are having issues with the amount of space assigned to them, either because their allotment has decreased substantially or their operations are expanding—for example, running up against storage limits for samples in the reference library.

Lastly, as regards the dissemination of outputs, MML could benefit from using its network of former postdocs as brand ambassadors, as was indicated in the 2017 review.<sup>1</sup> The research staff continues to make its mark in journals. The laboratory continues to hold an impressive number of convening activities. Its staff are very well represented on federal interagency groups such as the National Science and Technology Council (NSTC) and in the International Organization for Standards (ISO). MML could benefit from its permanent staff presenting more talks in various forums as a way of maintaining presence.

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<sup>1</sup> National Academies of Sciences, Engineering, and Medicine (NASEM), 2017, *An Assessment of the National Institute of Standards and Technology Material Measurement Laboratory: Fiscal Year 2017*, Washington, DC: The National Academies Press.

## CONCLUSIONS AND RECOMMENDATIONS FOR OFFICES AND DIVISIONS

### Office of Reference Materials

The Office of Reference Materials (ORM) manages the development, marketing, sales, and distribution of a vast inventory of SRMs that are utilized extensively by broad industry sectors including: food and nutrition, manufacturing, biotechnology and pharmaceuticals, and chemicals. The office functions as a stand-alone e-commerce business, which presents challenges that are different from those of the other units within MML. ORM relies on marketing and dissemination of their product offerings and has made great progress since 2017 in its e-commerce operations. Opportunities exist to further advance their critical role in the Nation's competitive economic position. Further opportunities to improve responsiveness to industry needs include packaging modernization, which may be facilitated by expanding strategic partnerships. There is tension in resource allocation associated with supporting existing SRMs and the development of new offerings that reflect the needs of emerging industrial sectors. The collaboration between ORM and other NIST units could be reinforced through strategic selection of industry-relevant projects that would be supported by the working capital fund.

**RECOMMENDATION 3-1:** The Office of Reference Materials (ORM) should plan and host a series of topic-focused workshops with participation from industry, academia, and other government organizations to benchmark and identify state-of-the-art business practices, e-commerce tools/platforms, marketing and sales operations, packaging, and other areas critical to its operations. As part of such an undertaking, ORM should assess the appropriateness and feasibility of outsourcing portions of its operations or the expanded use of public-private partnerships to increase efficiency of its operations including standard reference material fabrication, storage (inventory control), packaging, and other critical operations.

**RECOMMENDATION 3-2:** The Office of Reference Materials should develop processes and procedures to strategically select and prioritize the use of working capital funds toward high-demand products, which can maximize the throughput and return value; and examine methods to accelerate and evaluate the development of these new standard reference material products. The evaluation can be used to further promote and/or incentivize the MML division-level SRM development.

**RECOMMENDATION 3-3:** The Office of Reference Materials (ORM) should conduct informational symposia and workshops to better communicate the vital role that ORM plays in the mission of NIST and to highlight success stories. The office should also provide more systematic evaluation feedback and greater incentives for MML division staff to more effectively and efficiently develop new standard reference materials that are aligned with the needs of industry.

### Office of Data and Informatics

The Office of Data and Informatics (ODI) is a service-oriented organization whose mission is to provide leadership and expertise to meet the modern data challenges and leverage data-driven research opportunities for the MML and NIST scientific research data infrastructure. ODI is the principal outlet for SRD products across not only MML but NIST as a whole. MML produces about 90% of SRD NIST-wide.

ODI has a lead role in developing and piloting Laboratory Information Management Systems (LIMS). The successfully demonstrated pilot automates many key aspects of collecting and curating data



from electron microscopes. ODI has been successful in socializing the concept of a Data Management Plan (DMP) and continues to work in securing implementation by MML projects.

ODI views data as a key product resulting from the activities of MML and NIST. However, there is much to be done to establish this culture of viewing and valuing data as a key asset across NIST. While ODI has a vital role, ODI alone cannot make this transformation happen. That will require attention by MML management. More complete integration of ODI will impact priorities and plans both long and short term. The status of the LIMS initiative noted above offers a case study for MML and NIST on this opportunity.

Support for fundamental data activities is not always timely, and this has led to a lack of maintenance for a number of SRD products. Similarly, the Open Access to Research scientific data infrastructure work will need long-term support after this year when support from the Associate Director for Laboratory Programs ends. These instances suggest that the value of ODI's work is not universally recognized.

**RECOMMENDATION 4-1:** The Material Measurement Laboratory management should promote the concept of “data as an asset” and its associated culture within the Laboratory. With that understanding, management can be expected to advocate and support its adoption throughout the organization, resulting in increased professionalism within NIST, higher quality of output by NIST, increased impact of NIST products on the STEM world, and public perception of NIST as a leader.

Given its position and role in MML and NIST in general, the ODI, when properly leveraged and resourced (e.g., when it has funds to modernize SRD products), is in a unique position to advance the goals of not only MML but NIST more broadly. To achieve the potential of ODI will require an explicit effort at the laboratory level to bring about a cultural change that brings data as a product into the overall laboratory consciousness. The following recommendations outline the steps needed in such an effort.

**RECOMMENDATION 4-2:** The Office of Data and Informatics (ODI) should build out structures for enhancing divisional interactions. One concrete mechanism for this is to create tightly integrated multidisciplinary teams, which include ODI domain expertise as an integral part of a research team. The concept of “research software engineering” has been advocated as one such mechanism for creating research teams that can respond to the centrality of data and computation in a research activity.

Postdoctoral fellows are being used effectively in other organizational units within MML, however within ODI their use is limited. This is understandable given the service orientated nature of their mission. However, even within these confines, Postdocs could be used effectively both to advance the direct goals of the ODI, but more importantly to act as agents of culture change across the laboratory toward an awareness of data as a product. The ODI is already engaged in training with its programs in “software carpentry.”

**RECOMMENDATION 4-3:** The “software carpentry” program should be expanded to include rotations of postdocs through ODI for more extensive, hands-on guidance. In addition, identifying postdocs in the MML divisions with an understanding of the importance of sound computational techniques and establishing joint mentorship programs with those divisions and ODI would be beneficial.

**RECOMMENDATION 4-4:** The Material Measurement Laboratory should enhance engagement with creation/integration of reference materials.

## Materials Science and Engineering

The Materials Science and Engineering Division (MSED), conducts research in Thermodynamics and Kinetics, Mechanical Performance, Polymer and Complex Fluids, Functional Polymers, Polymer Processing, and Functional NanoMaterials that is among the best in the world. In addition the research groups are strongly coupled to their respective industries and provide unique resources in metrology. In particular the Thermodynamics and Kinetics group is respected worldwide for their expertise in computational materials science.

**FINDING:** The computational work of the Thermodynamics and Kinetics group is well ahead of many other entities outside of NIST.

**RECOMMENDATION 5-1:** The Materials Science and Engineering Division (MSED) should consider investment in additional high-performance computing resources to continue the comparative advantage the Thermodynamics and Kinetics group holds. In making such investments, MSED should maintain balance with empirical approaches.

While the equipment and facilities are very good to excellent, some equipment needs updating, necessitating a thoughtful, strategic equipment renewal process. Such a process would best emphasize “unique” equipment needed, even in areas such as electron microscopy, to differentiate MML from other federal labs. Strategic planning could incorporate the number of scientific staff and specific scientific expertise needed, equipment development needs, and standards development needs and prioritize all needed investments.

**RECOMMENDATION 5-2:** The Materials Science and Engineering Division should develop a clear articulation of a broad-based strategic plan of the division and state how that plan reflects the overarching strategic plan of the Material Measurement Laboratory.

MSED is fortunate to have high quality scientists and technical staff commitment to the organization. The technical team has the expertise required to accomplish programmatic objectives. The culture of MSED is such that post-docs appear inclined to stay at NIST if that opportunity is available.

MSED is addressing stakeholder needs especially at the high technological readiness levels (TRLs). Additionally there is adequate monitoring of stakeholder use and impact of program output. While there is good dissemination of results using print media, results from primary work in MML could be highlighted more.

**RECOMMENDATION 5-4:** The Material Measurement Laboratory should increase its activities aimed at communicating its accomplishments to its customers, collaborators, and audiences. This should include greater effort at highlighting results from the primary work of the laboratory. This could be accomplished using forms of media such as YouTube and improving the effectiveness of the NIST website by adding specific examples of unique and transformative contributions.

## Materials Measurement Science Division

The Materials Measurement Science Division (MMSD) conducts mission and fundamental research and provides state-of-the-art instrumentation methods, models, and software. Its SRM and SRD are used to validate methods and enable new technologies. The MMSD maintains a broad scientific portfolio encompassing five program areas: (1) Atomic Arrangement and Structure-Property Relationships; (2) Physical, Chemical and Mechanical Properties of Materials; (3) X-Ray Scattering and

Spectroscopy; (4) Materials and Metrology for Safety, Security and Forensics; and (5) Informatics and Artificial Intelligence for Materials Design. The Synchrotron Science Group maintains and supports synchrotron measurement capabilities as part of the U.S. Department of Energy's User Facilities program, primarily at the National Synchrotron Light Source II.

**FINDING:** The development, fabrication, and sale of standard reference materials and documentary standards are central to the mission of MMSD. MMSD has a broad client base for SRMs etc., but contacts are handled by other groups.

**RECOMMENDATION 6-1:** The Materials Measurement Science Division (MMSD) should increase the degree to which it utilizes its customers for feedback on new products and information with regard to emerging opportunities. To this end, the Material Measurement Laboratory should utilize a process for obtaining feedback. MMSD should increase its interaction with the offices managing sales of such products at NIST.

**FINDING:** The MMSD has the lowest female/male ratio compared with other divisions in the Material Measurement Laboratory.

**RECOMMENDATION 6-5:** The Materials Measurement Science Division (MMSD) should examine ways to recruit and retain greater numbers of female scientific staff. MMSD staff should all work to enhance the visibility of NIST as a career option through technical meeting/society activities and university interactions. All team members should ensure inclusiveness and assist with career development of the diverse workforce, including the careers of associates and post docs.

**FINDING:** The work of the MMSD is extremely dependent on access to state-of-the-art instrumentation. There were areas in which current new technologies are needed as a group moves into exciting new areas such as soft materials. Other instrumentation is aging and will need replacement in the near future (e.g., 3D atom probe instrumentation and electron microscopes). NIST extensively uses national user facilities beyond MMSD, particularly when instrument development is not a part of the project.

**RECOMMENDATION 6-6:** The Materials Measurement Science Division should prioritize the division's needs for upgrading/replacement of equipment and explore centralizing commonly used instrumentation at the division or laboratory level.

### **Biosystems and Biomaterials Division**

The NIST Biosystems and Biomaterials Division (BBD) is focused on four primary areas—engineering biology, advanced therapies, precision medicine, microbiome—with a drive to foster innovation and build confidence in quantitative biology and biomaterial measurements across government and industry in support of the bio-economy. Importantly, in response to the SARS-CoV-2 pandemic, BBD implemented targeted initiatives by redirecting resources in manpower, collaborations, and equipment.

BBD has five groups: complex microbial systems, biomarker and genomic sciences, biomaterials, cell systems, and cellular engineering. These cross-functional groups of scientists with expertise in materials, molecular biology, engineering, chemistry, microbiology, statistics and data management are working well together. The BBD team is highly successful in the development of advanced standards and innovative measurement technology to address the quantitative metrology needs of biological materials and processes.

BBD's primary products are measurement science and protocols, which are disseminated in publications, reference materials, and reference data—including, for example, Genome in a Bottle DNA, Cancer Biomarker EGFR (Epidermal Growth Factor Receptor) and MET, infectious disease antibodies and antigen, mixed pathogen DNA, reference materials for flow cytometry. Advanced living reference materials include, for example, genetically tagged yeast, microbial whole cell, human gut microbiome materials for validation of methodology. Also important is international biological lexicon standardization.

As a challenge, BBD has lost approximately 20 percent of its laboratory space, which negatively impacts program growth. The NIST Master Plan does include construction of a standard reference material facility for preparation and storage of biologic reference materials. Ensuring continued scientific interactions by addition of inside walkways to interconnect buildings would be beneficial.

Knowledge of complex biological systems is continually evolving with developing manufacturing methods for commercial biological materials. Interwoven knowledge in biology, chemistry, physics, math, and data/informatics is required. For BBD, this translates into a need for additional emphasis on colloidal science and thermodynamics, biofilm biochemists, and fluid mechanics.

**RECOMMENDATION 7-3:** The Material Measurement Laboratory should evaluate whether the square footage assigned the Biosystems and Biomaterials Division is commensurate with the division's current size and mission.

**RECOMMENDATION 7-4:** The Biosystems and Biomaterials Division should provide additional resources in thermodynamics, fluid mechanics, colloidal science, virology, immunology, microbiology, and bioinformatics in a manner commensurate with the increasing importance of these specialties.

**RECOMMENDATION 7-7:** The Biosystems and Biomaterials Division leadership should implement cross-training of staff with intent during each year to mitigate the effects of loss of key staff and ensure continuity.

### **Biomolecular Measurement Division**

The Biomolecular Measurement Division (BMD) has a comprehensive set of programs that builds upon the division's strengths in measurement and measurement research for:

- Biomolecular structure and function,
- Mass spectrometry data,
- Applied genetics,
- Bioprocess measurement, and
- Bioanalytical science.

BMD is technically strong compared to the state of the art (measured on a global basis); it has the needed technical expertise and is aware that the workforce needed to be much more diverse and was beginning to take action; adequate resources for current objectives, but will need to re-align and grow resources to address new areas—particularly in some areas of forensics, and separately, biophysical characterization of biologics and biologic particle sizing, and associated reference standards; and effectively disseminates its work through excellent and prolific publications, as well as biological reference materials.

BMD is fulfilling its mission, has good management, and good morale, with the exception of a desire of early career staff seeking more mentorship and recognition and that diversity of the workforce still needs to be achieved. The BMD is well organized, gave an impressive series of presentations,

collaborates with industry, and addresses key measurement and standards needs of government, academic researchers, and the rapidly growing biopharmaceutical sector. While BMD is managing closely its resources and maintaining productivity during the COVID-19 pandemic, future strengthening of its programs will likely require further attention to professional staffing needs as well as resources required to support these needs, particularly in the context of achieving a more diverse workforce and the enhanced work environment that would be anticipated to result. Overall, BMD should be recognized for its excellence in meeting current technical goals while positioning itself for future developments and inherent changes in the national and global landscape in biopharmaceutical, bioprocessing, biomolecular research, and renewable energy and bioproducts.

The applications of artificial intelligence (AI) and machine learning (ML) within BMD includes mass spectrometer (MS) spectra/databases, nuclear magnetic resonance (NMR) library contours, retention index analyses, forensics, and others. An AI/ML expert would likely provide novel insights into the embedding of these methods throughout the division and play an educational role.

**RECOMMENDATION 8-1:** The Biological Measurement Division (BMD) should evaluate its portfolio of expertise of staff with expertise in artificial intelligence and machine learning as applied to the measurement tools specifically in BMD. BMD might want to consider a joint hire with another division to leverage additional expertise and resources, or develop a more centralized collaboration model (i.e., community of practice) to make enhanced use of AI/ML expertise.

The majority of BMD's application areas are human based—that is, forensics, biotherapeutics, Chimeric antigen receptor T cells (CAR T cells), and so forth. Significant opportunities may be present in areas beyond that applied to humans and these include agriculture, veterinary science, biocatalysis, and environmental and marine research areas.

**RECOMMENDATION 8-2:** The Biological Measurement Division (BMD) should develop a strategy to assess agriculture, veterinary science, biocatalysis, and environmental and marine research areas as possible opportunities for growth and sources of additional collaborations and funding.

### Chemical Sciences Division

The work of the Chemical Sciences Division (CSD) ranges from inorganic and organic chemical metrology to biochemical and exposure science. They have had impressive recent successes including the Avogadro Project enabling the kilogram (kg) standard to be redefined, the development of FEASST (Free Energy and Advanced Sampling Simulation Toolkit), a suite of tools for enhancing bottom up prediction of physical and chemical properties, and the development and commercialization of a benchtop <sup>14</sup>C (carbon-14) instrument for applications in forensic analysis, radiocarbon dating, and emissions monitoring. Among its widely known capabilities, the division maintains and operates the biorepository for NIST, primarily of marine life, which has over 100,000 specimens with the ability to track long-term pollutants as well as identify emerging pollutants, and develops and applies measurement technologies for the analysis of gaseous samples that are critically important throughout industry, academia, and government. Further, taking a hard look at new activities to undertake, while maintaining or letting go of current activities, is critical to avoid overtaxing staff to increasingly do more with less. Finally, the possibility of clustering the groups into related subunits, or splitting the division to have more commonality within the division could be considered going forward.

There was a lack of connection between many of the activities in CSD as presented. There is an opportunity for CSD leadership to spend the time crafting a story that would highlight the connections between all teams, or bin the teams into groups in such a way as to provide some level of connection. It

may also be worth considering splitting the large groups that have more common alignment or putting some of the teams in other groups where there is alignment.

**RECOMMENDATION 9-1:** The Chemical Sciences Division (CSD) should consider administrative changes to give greater definition to connectivity among the division’s scientists, including binning the teams in CSD to make commonalities with other groups more apparent; and, as warranted, splitting larger divisions and aggregating the groups into new divisions where similarities are strongest.

Retraining was also seen as a challenge for many—to either stay abreast of the field, or to reinvent themselves into a new area. If a sabbatical program in which more senior NIST employees rotate to national laboratories, industry, or academia were possible and mutually beneficial, this could serve in retraining as well as increasing MML visibility. This “mixing” will undoubtedly lead to the attrition of some MML workers, but by increasing the visibility, may also have a two-way effect. Absent this, removing some of the barriers to working with outside people (industry) such as better accessibility to virtual teleconference software options is essential.

**RECOMMENDATION 9-2:** The Chemical Sciences Division should evaluate its portfolio to determine the fit to Material Measurement Laboratory’s (MML’s) strategy with a view toward adoption of a “steady state” economic model in which new costs are paid for by pruning existing operations. Alternatively, MML could adopt a “pay as you go” model in which they would add new programs, instrumentation, employees, and so forth as new funds become available, or by intentionally pursuing external funding in strategic areas.

There are opportunities for CSD to develop stronger ties with the pool of NIST postdoc alumni who will have now moved into positions in industry, government laboratories, small business, and academia. By celebrating this cadre of postdoc alumni, CSD would be clearly showing that there are pathways to successful careers for postdocs.

**RECOMMENDATION 9-4:** The Chemical Sciences Division (CSD) should remain in contact with postdoctoral (NRC and Associate) and other categories of associates who have left CSD as a way of collecting input on emerging areas of concern, problems of note, and feedback on the adoption and implementation of CSD and Material Measurement Laboratory efforts.

### Applied Chemicals and Materials

The Applied Chemicals and Materials Division (ACMD), located in Boulder, Colorado, characterizes the properties and structures of industrially important fluids and materials. Its work serves a diverse stakeholder community by providing innovative measurements and models and critically evaluated data with the goals of improving processes and products and developing new and improved standards.

Many of the individual projects are organized for either historical or administrative convenience, in contrast with unifying technical or methodological themes based on the MML mission statement. The division covers a number of long-standing “curator” functions such as the Charpy Verification Program and the REFPROP database (REFerence fluid thermodynamic and transport PROPERTIES), which are central to the NIST Mission but which dilute the scientific resources needed to maintain leadership in new areas of measurement science.

There have been no major new facilities for ACMD in the Boulder Campus or at least none were described to the panel. The major concern repeated numerous times was the housing of the programs in 50-year-old laboratories. This may be a legitimate concern but it is beyond the charge of the panel.

The ACMD dependence on a significant increase in associate staff for new programs may lead to potential program continuity issues as the tenure for short-term employees ends. It was apparent that tenure prospects have not been adequately conveyed to associates. ACMD would do best not to rely on increases in future associates to sustain additional program growth. As associates complete their tenure, new programs could be initiated and old programs ended.

If capital equipment replacement for aging tools is mission critical, then a priority list would need to be developed and provided to higher levels of the organization's management. ACMD noted potential equipment sources from the U.S. government surplus listings.

**RECOMMENDATION 10-1:** The Applied Chemicals and Materials Division should create a capital equipment replacement plan that considers also the requirements for space and ongoing maintenance.

ACMD has created significant impact with key SRDs and SRMs. The challenge for ACMD is to value their SRD/SRM portfolio so that new programs can be initiated, in particular programs that explore new solutions to legacy SRM strategies.

ACMD has SRD and SRM activities that utilize personnel resources to maintain legacy standards. Initiating new programs to examine replacement or improvement strategies for these standards activities would position ACMD at the forefront of the next generation of standards requirements. Properly valuing the SRD and SRM activities would create revenue to support such activities.

**RECOMMENDATION 10-2:** The Applied Chemicals and Materials Division should take steps to realize the true value of standard reference data and standard reference materials thereby enabling revenue for growth of new programs.

ACMD has the same breadth of commercial opportunities as does the MML, with an outstanding history of precision chemical, thermodynamic and mechanical property measurements. Virtually all of the projects within ACMD fit within divisions housed in Gaithersburg, yet it is not clear that the interaction between these two physically distant laboratories are as close as they might be in an era where virtual discussion is becoming the norm.

**RECOMMENDATION 10-3:** MML should (1) clearly define the Applied Chemicals and Materials Division's (ACMD's) mission and how ACMD aligns within the Material Measurement Laboratory mission; and (2) integrate teams more closely with corresponding efforts in NIST Gaithersburg facilities.

Highrisk project activity is one measure of the technical vitality of an organization. High-risk projects include vapor forensics for public safety and NMR and microwave techniques for thermodynamic property characterization.

**RECOMMENDATION 10-4:** The Applied Chemicals and Materials Division should continue to increase the number of high-risk projects.

# 1

## Introduction

Since 1959 the National Academies of Sciences, Engineering, and Medicine has annually assembled panels of experts—from academia, industry, medicine, and other scientific and engineering communities of practice—to assess the quality and effectiveness of the National Institute of Standards and Technology (NIST) measurements and standards laboratories, of which there are six,<sup>1</sup> as well as the adequacy of the laboratories’ resources. These reviews are conducted under contract at the request of the NIST.

In 2020, at the request of the Director of NIST, the National Academies formed the Panel on Review of the Material Measurement Laboratory of the National Institute of Standards and Technology (the “panel”), having earlier established the following statement of work:

The National Academies of Sciences, Engineering, and Medicine Panel on Review of the Material Measurement Laboratory at the National Institute of Standards and Technology will assess the scientific and technical work performed by the National Institute of Standards and Technology (NIST) Material Measurement Laboratory. The panel will review technical reports and technical program descriptions prepared by NIST staff and will visit the facilities of the NIST laboratory. The visit will include technical presentations by NIST staff, demonstrations of NIST projects, tours of NIST facilities, and discussions with NIST staff. The panel will deliberate findings, conclusions, and recommendations in a closed session panel meeting and will prepare a report summarizing its assessment of findings, conclusions, and recommendations.

The assessment shall be responsive to the charge from the NIST Director. The following are the criteria for the assessment:

1. The technical merit of the current laboratory program relative to current state-of-the-art programs worldwide;
2. The portfolio of scientific expertise as it supports the ability of the organization to achieve its stated objectives;
3. The adequacy of the laboratory budget, facilities, equipment, and human resources, as they affect the quality of the laboratory's technical programs; and
4. The effectiveness by which the laboratory disseminates its program outputs.

The panel’s review covered the six divisions and two offices that comprise the MML. The panel conducted its review remotely on September 9, 10, and 11, 2020, working in a synchronous fashion with MML staff and the NIST director, all of whom provided substantive and informative presentations. These presentations were interspersed with discussions between NIST staff and the panel. NIST staff further provided written responses to the panel’s queries.

The panel’s approach to the assessment relied on the experience, technical knowledge, and expertise of its members. Time constraints did not allow the panel to explore all aspects of the MML.

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<sup>1</sup> The six National Institute of Standards and Technology (NIST) laboratories are the Communications Technology Laboratory, the Engineering Laboratory, the Information Technology Laboratory, the Material Measurement Laboratory, the Physical Measurement Laboratory, and the Center for Neutron Research.



Rather, the panel focused on the research that the leadership of the MML chose to present to it and on a number of issues related to laboratory development that the panel identified as requiring particular attention. The panel's report includes recommendations that specify "who should do what" to address any determinations as to what might warrant action. The panel underpins the recommendations with salient examples of programs and projects that are intended collectively to portray an overall impression of the laboratory, while preserving useful suggestions specific to projects and programs.

To accomplish its mission, the panel reviewed the material provided by the MML prior to and during the review meeting. The choice of projects to be reviewed was made by the MML. The panel applied a largely qualitative approach to the assessment. Given the nonexhaustive nature of the review, the omission in this report of any particular MML project should not be interpreted as a negative reflection on the omitted project.

## 2

## Overview of the Material Measurement Laboratory

The Material Measurement Laboratory (MML) is one of six laboratories of NIST<sup>1</sup> and one of the NIST fundamental metrology laboratories.<sup>2</sup> The preponderance of MML activity occurs at the Gaithersburg, Maryland, campus, with more than 80 percent of its staff and associates. There is a substantial presence as well on the NIST Boulder, Colorado, campus. Smaller deployments are scattered across a further four sites, including the Institute for Bioscience and Biotechnology Research (IBBR)<sup>3</sup> in Rockville, Maryland; the Hollings Marine Laboratory (HML)<sup>4</sup> in Charleston, South Carolina; NIST Beamlines at the Brookhaven National Laboratory in Upton, New York; and the NIST Pacific Islands Program, in Oahu, Hawaii.

The MML “serves as the nation’s primary resource for advancing measurements essential to the chemical, biological, and materials sciences and related engineering disciplines.”<sup>5</sup> The work of the laboratory is concentrated in the chemical, biological, and materials sciences to “bring focus to the development of exceptional measurement science expertise and capabilities, reference products and standards, and data science and data dissemination capabilities.” The MML further identified programmatic opportunities it is pursuing which include the following: Bioeconomy and Engineering Biology, Data and Artificial Intelligence, and the Circular Economy.<sup>6</sup> The work of the MML is overall subsumed under three scientific and technical goals, which include (1) Measurement Science Excellence, (2) Measurement Service Excellence, and (3) Data Science and Data Management Capabilities, and a further two organizational goals, (4) strategic partnering and customer engagement and (5) organizational excellence.

There are six divisions and two offices. Five of the divisions—Materials Science and Engineering, Materials Measurement Science, Biosystems and Biomaterials, Biomolecular Measurement, and Chemical Sciences—are primarily located on the NIST campus in Gaithersburg, Maryland, are focused on research, as is a sixth, Applied Chemicals and Materials, located at the NIST Boulder campus at 325 Broadway. The two offices—Office of Reference Materials and the Office of Data and Informatics—are located on the Gaithersburg campus and are focused on measurement services. The MML identified challenges, including “Aging and Outdated Building Infrastructure” and “‘Large’ Equipment Needs and Uses.”<sup>7</sup>

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<sup>1</sup> The six National Institute of Standards and Technology (NIST) laboratories are the Communications Technology Laboratory, the Engineering Laboratory, the Information Technology Laboratory, the Material Measurement Laboratory, the Physical Measurement Laboratory, and the Center for Neutron Research.

<sup>2</sup> Walter Copan, “Welcome to NIST,” presentation to the panel, September 9, 2020.

<sup>3</sup> A joint research enterprise between University of Maryland and NIST.

<sup>4</sup> A partnership between NIST, the National Oceanic and Atmospheric Administration, the South Carolina Department of Natural Resources, the College of Charleston, and the Medical University of South Carolina.

<sup>5</sup> NIST Material Measurement Laboratory, 2020, “National Academies of Sciences, Engineering, and Medicine: 2020 Assessment Read-Ahead Materials for September 9-11, 2020,” Gaithersburg, MD.

<sup>6</sup> *Ibid.*, p. 2.

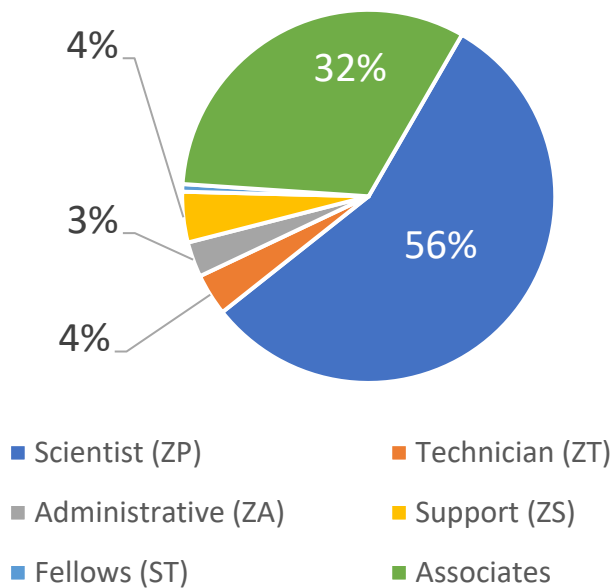
<sup>7</sup> *Ibid.*

**TABLE 2.1** MML Annual Budgets (\$000)

Budget Type	FY2017	FY2018	FY2019	FY2020 <sup>a</sup>
Congressional Appropriation (STRS)	128,728	138,854	137,140	142,325
Measurement Services	34,325	35,839	35,485	35,962
Other Agency Agreements (OA)	24,238	25,320	22,659	21,077
Total	187,291	200,013	195,284	199,364

<sup>a</sup> Estimated.

NOTE: STRS = Scientific and Technical Research and Services.



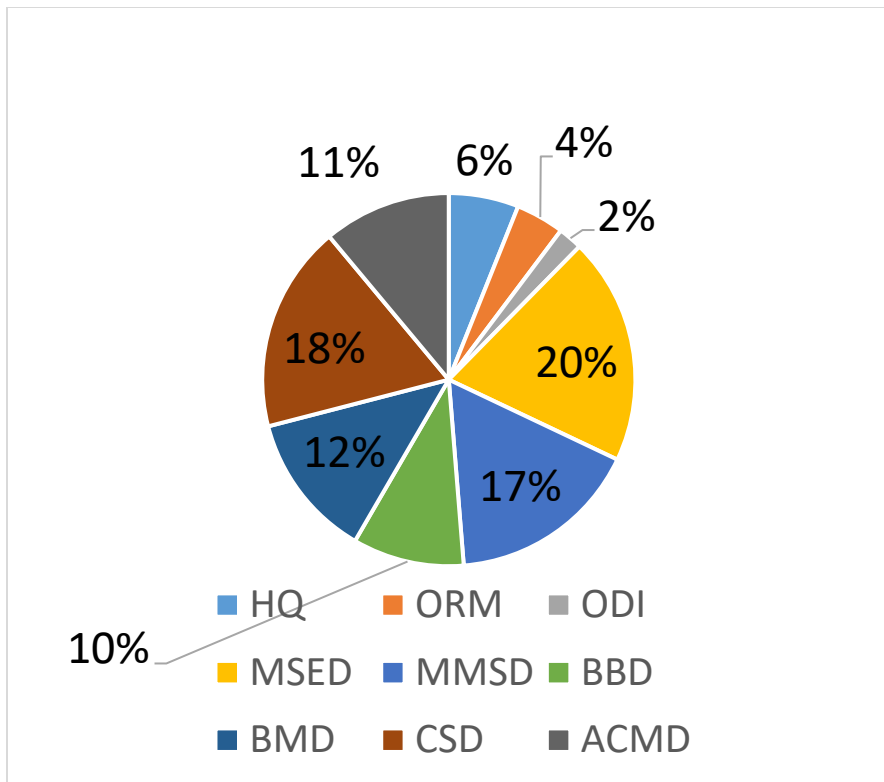
**FIGURE 2.1** Staff by type.

The budget authority for the MML was \$195 million in fiscal year (FY) 2019. Details and prior-year funding appear in Table 2.1.

As of April 2020, there were 858 staff in the MML, including both federal employees and associates. The latter category includes roughly one-third of this number and includes students, post-doctoral associates, and contractors (see Figure 2.1). The allocation of staff to the six divisions, two offices, and the headquarters unit are shown in Figure 2.2.

While data on underrepresented minorities among staff were not readily available, for NIST overall roughly 1 in 11 STs (fellows) were minorities, and within the ZP (scientist) category, 1 in 6 at Level V were minorities, and at Levels III and IV it was 1 in 4.<sup>8</sup>

<sup>8</sup> NIST, 2019, “Inclusivity at NIST: Recent Actions Supporting Equity in Career Advancement at NIST,” presentation to the Visiting Committee on Advanced Technology, October 24, Gaithersburg, MD.



**FIGURE 2.2** Percent of staff in each organizational unit of the Material Measurement Laboratory. NOTE: HQ = Headquarters; ORM = Office of Reference Materials; ODI = Office of Data and Informatics; MSED = Materials Science and Engineering Division; MMSD = Materials Measurement Science Division; BBD = Biosystems and Biomaterials Division; BMD = Biomolecular Measurement Division; CSD = Chemical Sciences Division; ACMD = Applied Chemicals and Materials Division.

### 3

## Office of Reference Materials

The Office of Reference Materials (ORM) manages business operations, administrative oversight, product sales, and technical support for the NIST Standard Reference Material (SRM) program. The MML produces about 90 percent of the total SRM NIST-wide.<sup>1</sup> The office houses associated physical and cyber infrastructure to produce, package, store, and market SRM products and then sell them to customers worldwide. There were significant improvements to the ORM e-business platform that have increased productivity, efficiency, and customer relations. The ORM delivers its mission successfully with direct alignment of the NIST mission to support U.S. industry and commerce.

### ASSESSMENT OF TECHNICAL PROGRAMS

In contrast to the MML divisions, ORM functions as a stand-alone e-commerce business operating within the constraints of a federal agency. This presents unique business, staffing, and technical challenges that are differentiated from other units within the MML. The assessment of ORM's technical programs thus differs from that which applies to the divisions.

The ORM can list a number of accomplishments that are aligned with its mission and programmatic goals. The number of sales of SRM products totals approximately 32,000 units per year, resulting in roughly \$21.5 million in income. The sales group of six people and one group leader fields more than 10,000 customer inquiries per year, including requests for quotes and technical information. More than 10,000 orders are shipped each year. The top 15 sales products for fiscal year 2019 are show in decreasing order of sales.

The customer base for ORM products consists of 52 percent, U.S. industry; 45 percent, international industry; 2 percent, U.S. federal government; 2 percent, foreign government; and 1 percent, state and local governments across all major industrial sectors. International sales have been increasing steadily and now account for nearly half of all sales.

### Opportunities and Challenges

Packaging and storage concerns are a significant risk to the current operations and business model of ORM. The lack of sufficient facilities specifically related to bio-economy related SRMs limits ORM from moving into emerging markets that require good manufacturing practices (GMP) and other requirements. Product packaging and distribution is a significant fraction of ORM activities. Yet, ORM lacks expertise and partnerships for new packaging capabilities needed for anticipated products. Outreach

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<sup>1</sup> Steven Choquette, National Institute of Standards and Technology, 2020, "NIST/Office of Reference Materials Overview," presentation to the panel, September 9.

**TABLE 3.2** Top Selling Standard Reference Materials in Fiscal Year 2019

SRM	Name	Units Sold
2096	High-Energy Charpy V-Notch Specimens (NIST-Verification, 8-mm Striker)	1,632
2092	Low-Energy Charpy V-Notch Specimens (NIST-Verification, 8-mm Striker)	1,627
8671	NISTmAb, Humanized IgG1K Monoclonal Antibody	1,101
84l	Potassium Hydrogen Phthalate Acidimetric Primary Standard	712
1849a	Infant/Adult Nutritional Formula I (milk-based)	607
1640a	Trace Elements in Natural Water	551
114q	Portland Cement Fineness Standard	480
1921b	Infrared Transmission Wavelength/Wavenumber Standard	419
927e	Bovine Serum Albumin (7 % Solution) (Total Protein Standard)	362
1976c	Instrument Response Standard for X-Ray Powder Diffraction	353
17f	Sucrose (Optical Rotation)	325
46h	Portland Cement Fineness Standard	314
1976b	Instrument Response Standard for X-Ray Powder Diffraction	309
1950	Metabolites in Frozen Human Plasma	301
2709a	San Joaquin Soil Baseline Trace Element Concentrations	283

NOTE: SRM is the inventory number (left-most column).

and partnerships with industry leaders may contribute to innovative solutions for ORM packaging and e-business platform modernization. Lastly, ORM briefed on storage infrastructure being at or close to capacity, particularly in the context of unstable products that require special handling, such as cold storage.

**RECOMMENDATION 3-1:** The Office of Reference Materials (ORM) should plan and host a series of topic-focused workshops with participation from industry, academia, and other government organizations to benchmark and identify state-of-the-art business practices, e-commerce tools/platforms, marketing and sales operations, packaging, and other areas critical to its operations. As part of such an undertaking, ORM should assess the appropriateness and feasibility of outsourcing portions of its operations or the expanded use of public-private partnerships to increase efficiency of its operations including standard reference material fabrication, storage (inventory control), packaging, and other critical operations.

### PORTFOLIO OF SCIENTIFIC EXPERTISE

The portfolio of expertise of ORM is aligned with its mission as a stand-alone business unit and does not lend itself to direct comparison to other MML divisions. Of the 37 staff members, 32 percent are scientists, 24 percent are technicians, 35 percent provide administrative or other program support, and a further 8 percent are associates. This make-up is thus distinct from that of the divisions. The scientific and technical staff collaborate with peers in research divisions to produce and document existing SRMs and perform the necessary research and measurements to create new SRM products as they are needed by industrial customers.

## **Accomplishments**

ORM successfully manages the development, marketing, sales, and distribution of a vast inventory of SRMs to national and international customers. These SRMs are procured directly from ORM and utilized extensively by industry in broad sectors, including food and nutrition, manufacturing, biotechnology and pharmaceuticals, and chemicals. Many of the SRMs are long-standing offerings that are augmented by new SRMs developed in partnership with other units across the MML via a Working Capital Fund.

## **Opportunities and Challenges**

International competitors are utilizing and leveraging the growth of SRM market to gain competitive advantage in emerging industry sectors, and ORM exists in an increasingly competitive market. ORM balances the market demand for recertifying existing products with the development of new SRMs in partnership with the MML research divisions. This tension stretches resources and may hinder ORM's ability to anticipate and respond to industry needs for SRMs in time—particularly for emerging growth sectors. ORM recognizes the need for better strategic selection, focused investment, and shorter development times for new SRM products. Opportunities exist at the MML level to promote and incentivize the development of new SRMs through division(s)—ORM partnerships that align with the needs of industry.

**RECOMMENDATION 3-2:** The Office of Reference Materials should develop processes and procedures to strategically select and prioritize the use of working capital funds toward high-demand products, which can maximize the throughput and return value; and examine methods to accelerate and evaluate the development of these new standard reference material products. The evaluation can be used to further promote and/or incentivize the MML division-level SRM development.

## **ADEQUACY OF FACILITIES, EQUIPMENT AND HUMAN RESOURCES**

ORM relies on the analytical and research facilities in 18 divisions across four NIST laboratories to make appropriate measurements in support of mission delivery. ORM has facilities and equipment that support SRM preparation, packaging, and shipping. The office is allocated a 20,000-square foot building for storage (approximately 800,000 units in bulk and packed), sample preparation, and shipping operations. Some products require controlled temperatures while stored, and ORM maintains close to sixty  $-80^{\circ}\text{C}$  freezers, seven walk-in  $-20^{\circ}\text{C}$  freezers and four walk-in  $4^{\circ}\text{C}$  refrigerators. In support of the growing need for biological SRMs, ORM has two 40-liter liquid  $\text{N}_2$  (nitrogen) freezers to store tissue samples from the Hollings Marine Laboratory.

## **DISSEMINATION OF OUTPUTS**

ORM relies on marketing and dissemination of its product offerings, and the office has made great progress since 2017 in its e-commerce operations and platforms. Yet, opportunities exist to better communicate its products, engage the community for input on new products, outreach to broader future science, technology, engineering, and mathematics (STEM) generations, and advance its critical role in the nation's competitive economic position. Internally, it appears that MML staff members have a varied understanding of SRM business operations. Incentives for greater participation in development of SRMs in MML division staff were not readily apparent. Externally, there are extensive partnerships and

engagement with industry and other SRM producers worldwide. These are important, yet largely transactional with limited specific strategic engagements. There are significant opportunities for MML and ORM to increase strategic engagements to improve marketing, especially on the e-commerce business context, of existing programs and garnering input for emerging product needs.

**RECOMMENDATION 3-3:** The Office of Reference Materials (ORM) should conduct informational symposia and workshops to better communicate the vital role that ORM plays in the mission of NIST and to highlight success stories. The office should also provide more systematic evaluation feedback and greater incentives for MML division staff to more effectively and efficiently develop new standard reference materials that are aligned with the needs of industry.



## 4

# Office of Data and Informatics

## INTRODUCTION

The Office of Data and Informatics (ODI) is an office within the Material Measurement Laboratory (MML). ODI is a service-oriented organization whose mission is to provide leadership and expertise to meet modern data challenges and leverage data-driven research opportunities for the MML and NIST scientific research data infrastructure. This helps NIST scientists optimize the discoverability, usability, and interoperability of their data products. ODI contributes to the overall mission of the MML and NIST by providing guidance in best practices and resources that optimize the creation and use of data products. They provide guidance, assistance, and resources for the biological, chemical, and materials work of the MML. In this role, ODI coordinates across MML laboratory domain experts and other data specialists at NIST.<sup>1</sup>

The ODI is focused on four functional areas: (1) distribution and curation of standard reference data (SRD); (2) research data management, preservation and dissemination; (3) in-house consultation services on informatics and analytics methods and tools; and (4) open data/open science community engagement.<sup>2</sup> In fiscal year (FY) 2020, ODI's budget was \$4.744 million, 20 percent of which came from revenues from SRD services connected with fulfillment of 2,600 ecommerce orders.

Current staffing of ODI is 18 full-time equivalents (FTEs), which includes the director and a senior advisor, 6.5 technical staff in the Data Services Group, 6 technical staff and 2 contractors in the Data Sciences Group, 1.5 FTE of administrative support, and several affiliated staff not directly assigned to ODI.

## ASSESSMENT OF TECHNICAL PROGRAMS

### Accomplishments

ODI is the principal outlet for SRD products across not only the MML but NIST as a whole. MML produces about 90 percent of SRD NIST-wide. It delivers SRD products to customers outside NIST, collect license revenue under copyright laws, and remit the funds to other NIST organizations to support the development, maintenance, and enhancement of SRD products.

It serves as the repository for SRD artifacts, safeguarding their technical and legal integrity. The repository also serves as the way for the public to browse and shop for SRD products. ODI recently started to migrate to Salesforce.com to better manage this activity.

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<sup>1</sup> Robert Hanisch, National Institute of Standards and Technology (NIST), 2020, "Office of Data and Informatics, Division 641: Overview," presentation to the panel, September 9.

<sup>2</sup> NIST Material Measurement Laboratory (MML), 2020, "National Academies of Sciences, Engineering, and Medicine: 2020 Assessment Read-Ahead Materials for September 9-11, 2020," Gaithersburg, MD.

ODI has a lead role in developing and piloting laboratory information management systems (LIMS). The successfully demonstrated pilot automates many key aspects of collecting and curating data from electron microscopes. LIMS resulted in more productivity for researchers using the complex instruments and control of their data through collaboration and publishing results.

ODI plays a lead role in advocating data management plans (DMPs). Under a directive from the Office of Science and Technology Policy (OSTP),<sup>3</sup> NIST is supposed to create DMPs for projects that summarize how the data are to be gathered, utilized, analyzed, disseminated, and preserved. ODI has been successful in socializing the concept of DMP and continues to work in securing implementation by MML projects.

ODI also plays a lead role in developing and advancing the concept of data frameworks. More ambitious than DMPs, the data framework considers the entire life cycle of data artifacts, from planning and requirements establishment, data creation/collection, use and analysis, curation, sharing, protection, access, archiving, and ultimate deaccession. ODI's efforts for data frameworks are both internal to the MML and NIST, and external, with ODI taking a leadership role on this subject to the larger STEM community.

### **Challenges and Opportunities**

The challenges and opportunities for the technical programs will be discussed below, jointly with those of the portfolio of scientific expertise.

## **PORTFOLIO OF SCIENTIFIC EXPERTISE**

### **Accomplishments**

The accomplishments with respect to the portfolio of scientific expertise were discussed above, jointly with those of the technical programs.

### **Challenges and Opportunities**

Data is central to virtually every activity across the MML and NIST. Best practices for data collection, curation, collaboration, transformation, analysis, protection, archiving, and life-cycle management become ever more crucial to the performance of STEM organizations. ODI's role is to advocate, advise, consult, build and curate tools, and provide training in support of this mission.

ODI views data as a key product resulting from the activities of the MML and NIST, and therefore as a key asset of the organization. One could say that ODI has the ambition to foster a culture in which data as a pervasive asset becomes established in the research and development activities of every group, division, and laboratory at NIST, embraced and advocated at all levels of management.

There is much to be done to establish this culture of viewing and valuing data as a key asset across NIST. While ODI has a vital role, ODI alone cannot make this transformation happen. That will require attention by MML and NIST management to the issue. It will impact priorities and plans both long and short term.

The status of the LIMS initiative offers a case study for the MML and NIST on this opportunity. In collaboration with an active research group, ODI helped create a successful pilot LIMS implementation for certain electron microscopes, as noted above. That success creates the opportunity to move LIMS

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<sup>3</sup> John Holdren, Director, Office of Science and Technology Policy, 2013, "Memorandum for the Heads of Executive Departments and Agencies," February 22, [https://obamawhitehouse.archives.gov/sites/default/files/microsites/ostp/ostp\\_public\\_access\\_memo\\_2013.pdf](https://obamawhitehouse.archives.gov/sites/default/files/microsites/ostp/ostp_public_access_memo_2013.pdf).

from pilot to production status, to expand the software to cover more electron microscope types, and to build LIMS for other types of complex instruments. However, realizing this potential will necessitate changes in the priorities and programs from current plans, not just by ODI, but more broadly in other MML organizations. This is clearly something that ODI cannot be expected to accomplish on its own.

Support for fundamental data activities is not always timely, and this has led to a lack of maintenance for a number of SRD products.<sup>4</sup> ODI was able to initiate seven SRD enhancement projects using a one-time allocation of funds. The need to assess data quality on an ongoing basis suggests that ongoing funding would be better. Similarly, the Open Access to Research scientific data infrastructure work will need long-term support after this year when support from Associate Directory for Laboratory Programs ends. These instances suggest that the value of ODIs work is not universally recognized, notwithstanding some of the successes ODI has had at its own initiative to embed staff in other NIST organizational units (see discussion below in “Dissemination of Outputs”).

**RECOMMENDATION 4-1:** The Material Measurement Laboratory management should promote the concept of “data as an asset” and its associated culture within the Laboratory. With that understanding, management can be expected to advocate and support its adoption throughout the organization, resulting in increased professionalism within NIST, higher quality of output by NIST, increased impact of NIST products on the STEM world, and public perception of NIST as a leader.

## ADEQUACY OF FACILITIES, EQUIPMENT AND HUMAN RESOURCES

### Accomplishments

ODI seemed to have made serious progress in achieving the goals in response from the 2017 report. In the response to the 2017 review,<sup>5</sup> ODI had proposed to push for laboratory-driven science involving instrumentation and detectors and analytics. ODI has introduced efforts to embed data-driven metrology into the research workflow at NIST. LIMS capabilities at NIST have advanced significantly through establishment of a network.

The SRD program is providing a good service with a sustainable financial model for industry. The research data framework has a strong outreach program.

### Challenges and Opportunities

ODI could benefit from a sustainment strategy of meeting the goals in its LIMS efforts to ensure that any progress made in the past 3 years is not lost. The challenges include the following:

- A diverse set of needs across the laboratory, with no one system meeting everyone’s needs.
- Most divisions lack a DMP and continue to work through requirements and workflows.
- LIMS is an unfunded effort.

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<sup>4</sup> NIST MML, 2020, “National Academies of Sciences, Engineering, and Medicine: 2020 Assessment Read-Ahead Materials for September 9-11, 2020,” Gaithersburg, MD, p. 52.

<sup>5</sup> National Academies of Sciences, Engineering, and Medicine (NASEM), 2017, *An Assessment of the National Institute of Standards and Technology Material Measurement Laboratory: Fiscal Year 2017*, Washington, DC: The National Academies Press.

ODI needs software engineers, as there is minimal expertise across NIST for scientific data systems design and architecture. A high level of security is required for NIST, and gate keeping for deployments, requirements, and design are not available.

To help grow and sustain LIMS efforts, it may be desirable to establish informatics/data tools that enable one to fuse data across instrumentation. Another potential opportunity is to link to computational infrastructure to connect characterization and simulation studies. Further opportunities have been identified by ODI, including the completion of LIMS requirements, design, and workflows to level of support for roll-out across division projects.

## DISSEMINATION OF OUTPUTS

### Accomplishments

ODI has been active in numerous outreach efforts such as the Project Open Data Cloud-First strategy, an enhanced science data portal and an open-source code base hosted on github/USNISTGOV. ODI has been active in both national and international scientific efforts, including CODATA and OSTP subcommittees. The Informatics and Analytics program area has embedded staff in different NIST collaborations and introduced seminars and sponsored membership in The Carpentries,<sup>6</sup> a non-profit organization that provides training in coding and data science skills (i.e., “software carpentry”).<sup>7</sup> NIST is now well positioned to meet the new *Federal Data Strategy 2020 Action Plan*.<sup>8</sup>

### Challenges and Opportunities

The cultural acceptance of doing data-driven research is still a challenge. Scientific researchers not familiar with data analytical techniques still question why it is necessary to track and keep data. The challenges acknowledged in the 2017 report seem to persist. Initial efforts toward DMPs were uneven, and staff generally consider DMPs to be an administrative burden with no real benefit.

Unfortunately, there is still no one-size-fits-all LIMS solution for the diversity of data and operational modes present within MML; however, by building and reutilizing and by working in collaboration with technical staff in each division—perhaps by the latter assigning a data steward with a partial FTE—progress can be made.

With respect to SRD, copyright issues could interfere with the business model. NIST will need to consider how to address the challenge of how does one continue in an “open data” environment. A strategy needs to be established on how to maintain the financial model but still meet the spirit and intent of open access in the scientific community.

With the unique resource available through the NIST postdoc program, ODI may want to include informatics training of post docs by setting up laboratory rotations with the other divisions. This may help to expand the role of informatics/data science tools as more than just a service but a critical value-added component in research.

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<sup>6</sup> For further information, see The Carpentries, “The Carpentries,” <https://carpentries.org/>, accessed April 26, 2021.

<sup>7</sup> NIST MML, 2020, “National Academies of Sciences, Engineering, and Medicine: 2020 Assessment Read-Ahead Materials for September 9-11, 2020,” Gaithersburg, MD, p. 48.

<sup>8</sup> For further information, see Federal CDO Council, “2020 Action Plan,” updated May 14, 2020, <https://strategy.data.gov/action-plan/>.

## OVERALL CONCLUSIONS AND RECOMMENDATIONS

It is widely recognized that data is central to advances in science and engineering and is critical to the competitiveness of U.S. industry. Given its position and role in the MML and NIST in general, ODI, when properly leveraged and resourced (e.g., when it has funds to modernize SRD products), is in a unique position to advance the goals of not only the MML but NIST more broadly. To achieve this potential, ODI will require an explicit effort at the laboratory level to bring about a cultural change that brings data as a product into the overall laboratory consciousness (see Recommendation 4-1). ODI's current activities, such as development of LIMS systems to provide the institutional infrastructure, mentorship and training will accelerate this culture shift.

The following recommendations are intended to facilitate this shift.

**RECOMMENDATION 4-2:** The Office of Data and Informatics (ODI) should build out structures for enhancing divisional interactions. One concrete mechanism for this is to create tightly integrated multidisciplinary teams, which include ODI domain expertise as an integral part of a research team. The concept of “research software engineering” has been advocated as one such mechanism for creating research teams that can respond to the centrality of data and computation in a research activity.

**FINDING:** Postdoctoral fellows are being used effectively in other organizational units within the MML, however within ODI their use is limited. This is understandable given the service-orientated nature of their mission. However, even within these confines, postdocs could be used effectively both to advance the direct goals of ODI, but more importantly to act as agents of culture change across the laboratory toward an awareness of data as a product. ODI is already engaged in training with its programs in “software carpentry.”

**RECOMMENDATION 4-3:** The “software carpentry” program should be expanded to include rotations of postdocs through ODI for more extensive, hands-on guidance. In addition, identifying postdocs in the MML divisions with an understanding of the importance of sound computational techniques and establishing joint mentorship programs with those divisions and ODI would be beneficial.

**RECOMMENDATION 4-4:** The Material Measurement Laboratory should enhance engagement with creation/integration of reference materials.

## 5

**Materials Science and Engineering****INTRODUCTION**

The Materials Science and Engineering Division (MSED) supports the NIST Material Measurement Laboratory (MML) activities in advanced manufacturing (including Materials Genome Initiative 2.0, Additive Manufacturing and Biomanufacturing) and in Quantum Materials with the Physical Measurement Laboratory. The division also has programs in nano lithography, sustainability, and dental materials. Many of the topics are crosscutting between programs, and some programs are shared with other divisions of NIST. MSED made six presentations to the panel, including the following: Thermodynamics and Kinetics Group, the Mechanical Performance Group, Polymers and Complex Fluids Group, Functional Polymers Group, Polymers Processing Group, and the Functional Nanostructured Materials Group.

In MSED, there are a total of 151 staff members, which includes permanent staff, postdoctoral fellows, associates, and administrative support. In 2017, the staff was 168, indicating the total staff count has decreased by 17 persons over the past 3 years. Most of the reductions in staff are in the category of associate postdocs, which went from 44 to 27 during the past 3 years. (Associate postdocs are funded not by NIST but by another sponsoring organization.) MSED staff represents about 19 percent of the total MML staff. The budget for 2020 was \$27.457 million, which included indirect cost.<sup>1</sup> The budget is essentially flat as compared to 2017 when the panel last reviewed the laboratory.<sup>2</sup>

**ASSESSMENT OF TECHNICAL PROGRAMS****Accomplishments**

MSED's Thermodynamics and Kinetics Group is respected world-wide for its expertise in computational materials science. Its primary goal is to reduce the cost and time of alloy development. In addition to staff expertise with computational tools (e.g., CALPHAD, etc.), its suite of data repositories (e.g. phase-based data center, interatomic potentials repository) are becoming highly valued in the academic and industrial research communities.

Good models without solid empirical validation and downstream applications have limited value. Therefore, the group has empirical laboratory facilities to cast and process metal alloys. As additive manufacturing and other far-from-equilibrium processes become more commonplace, it will be important to strategically evaluate and upgrade laboratory equipment to keep a balance between the synergistic

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<sup>1</sup> Mark R. VanLandingham and John E. Bonevich, National Institute of Standards and Technology (NIST), 2020, "Materials Science and Engineering Division," presentation to the panel, September 9.

<sup>2</sup> National Academies of Sciences, Engineering, and Medicine, 2017, *An Assessment of the National Institute of Standards and Technology Material Measurement Laboratory: Fiscal Year 2017*, Washington, DC: The National Academies Press.

computational and empirical approaches. One example is adding a high-temperature, gas-cooled vacuum furnace to improve non-equilibrium capability. The group has a very solid track record of metallurgical alloy development, such as in Ni and Co superalloys, and coinage alloys. Of note is its recent work on 17-4 stainless in additive manufacturing. 17-4 is a very common, higher-strength, martensitic stainless steel that has wide application nationally. However, when it is processed far from equilibrium by using additive manufacturing techniques, 17-4 stainless has dramatically different microstructure and resulting properties compared to traditionally processed material. The group is working on the alloy design of this material to provide more stable microstructure and properties when it is used in additive manufacturing. This far-from-equilibrium work is evidence of the group's understanding and supporting new metallurgical engineering directions in this field. The group is also supporting computational polymers research, which is commendable. This is very complementary to the work in metals and will likely benefit longer-term research in industrially important processes where metals and polymers interact, such as paints and coatings.

**FINDING:** The computational work of the Thermodynamics and Kinetics Group is well ahead of many other entities outside of NIST.

**RECOMMENDATION 5-1:** The Materials Science and Engineering Division (MSED) should consider investment in additional high-performance computing resources to continue the comparative advantage the Thermodynamics and Kinetics group holds. In making such investments, MSED should maintain balance with empirical approaches.

The Polymers and Complex Fluids Group spans a wide range of scientific technologies and applications. A key to the success of this group is having and developing new analytical techniques to understand and analyze materials. In support of this, eight pieces of analytical equipment have been acquired since 2017. Such excellent equipment is one part of the equation, but also needed are dedicated users who receive cross-training to continue to excel in their application on a long-term basis. To this end, it will be important to support the integrated polymer analytics cross-functional group project in 2021. Understanding macromolecular architectures and polymer degradation mechanisms and their quantification are a strength of the group's work in this area. The group also works hard on using polymer science in supporting other areas of technology, such as their exceptional carbon nanotube separation technology. The group overtly makes a substantial effort to identify the overlap between fundamental science and industrial need and to plan strategically based on this information. Labor, budget, and priorities are set on an annual basis.

Within the Mechanical Performance Group, the NIST Center for Automotive Lightweighting addresses a significant national need. The U.S. transportation sector consumes more energy and generates more carbon dioxide (CO<sub>2</sub>) than buildings or industry, the other energy end-use categories. For personal transportation, lightweighting offers a direct path to meaningful energy savings and CO<sub>2</sub> reduction in the short-term (next 5 years) and potentially long-term. One of the immediate impacts has been in assessing sheet metal forming. This program, and associated consortia, specializes in multi-axial, multi-strain path, and high-strain-rate measurement and testing that is traditionally more difficult for individual companies to perform and model in a standardized manner. Two new approaches to cruciform testing using built-up specimens and thick-to-thin samples to better localize deformation have particular utility for automotive sheet designs and subsequent lightweighting. Measurement of macro and micro stress and high-speed thermographic measurements when performing tests is among the best in the world and brings a scientific level of insight to these mechanical testing methodologies. Digital Image Correlation (DIC) using both speckle and patterning provides empirical data to validate computational forming models. The program is to be commended for the 2020 Numisheet benchmarking study<sup>3</sup> and its structured links to industry that

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<sup>3</sup> NIST, 2020, "2020 Numisheet Benchmark Study Uniaxial Tensile Tests Summary," April 29, <https://www.nist.gov/publications/2020-numisheet-benchmark-study-uniaxial-tensile-tests-summary>.

enable rapid dissemination of its work product into the marketplace. In the area of composites, studying fiber fragmentation with Dow and Ford is an enabler of cost-effective, high strength-to-weight ratio composite adoption in automotive and light truck applications. It should be noted that having local machine shop capability to expedite test method development is a best practice and increases efficiency in this area.

Measurement of hardness and coating thickness is essential to many products that are widely used in the economy (e.g., engine components, bearings). The National Metrology Institute capacity of MML works with numerous influential companies to assure that standards and test methods (e.g., Knoop and Vickers) are accurately and properly transitioned into the marketplace. The importance of this work to the economy cannot be understated.

Additive manufacturing is a hot topic in the field of materials science and engineering. Almost every governmental laboratory in the nation has some activity in this area. It is critical to differentiate the work being conducted at NIST, as compared to many of these other laboratories and industry. NIST is “laser-focused” on obtaining numerous, physics-based, quantitative, in situ measurements of what is happening in the “weld” pool. This is absolutely essential for several reasons, and the depth of this undertaking is what sets NIST apart from other organizations. The first reason that this work is essential is that accurate in situ measurements enable active process feedback and closed-loop machine control for reproducible and superior part quality. Second, these measurements also enable the next generation of manufacturing and data analytics to occur in this field (industry 4.0 approach). Third, it provides quantitative, accurate numerical data that can be both integrated into computational modeling efforts and used to validate computational models. Finally, these measurements provide a much deeper understanding of the physics of the additive manufacturing process, which will enable both more statistically reliable parts (and increased applications) and future technical process advancement in this area. Additive manufacturing is transitioning from a “let’s just set our process controls and see what we get after the fact” approach to a “thoughtful, modeled, physics-based, quantitative in situ measurement and closed-loop feedback control” approach. The MML is providing leadership in this effort, and its own program is among the best in the world. The MML is also to be commended for their efforts in AM Bench and One NIST, which unites the technical community and starts solid data stewardship in the field of additive manufacturing.

The Functional Polymers Group works in three areas—Polymer Transport, Polymer Matrix Composites, and Polymer Mechanics. In alignment with the overall mission of NIST, industry is the group’s number one customer, but they also interact with government agencies. Recently, the group filed six patent disclosures, four patent applications, and has three active CRADAs (Cooperative Research and Development Agreements). The majority of this work on the innovation continuum starts at lower technology readiness levels (TRLs)<sup>4</sup> where they continue the efforts of academics and continue through higher TRLs up to the point that they enable commercial products (e.g., football helmet energy mitigation products, membrane technology, ballistic mitigation products). This range of TRL efforts appropriately keeps them balanced on both the science of polymers and the engineering applications that benefit the economy. This group is to be commended for thoughtfully and actively managing this balance between science and engineering. Of particular note is its work starting at the molecular level of understanding for enabling high strain rate and short-time-scale mechanics applications (e.g., impact mitigation, noise mitigation).

Work on polymer matrix composites tends to be focused on fiber–matrix and filler–matrix interactions, which are essential for high strength-to-weight-ratio applications in real-world environmental applications. Analytical techniques and the associated equipment to perform measurements

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<sup>4</sup> A number of agencies maintain their own TRL scale as a measure of the maturity of technology as it progresses toward deployment. The TRL metric developed by NASA is often cited; see NASA, “Technology Readiness Level,” updated October 28, 2012, [https://www.nasa.gov/directorates/heo/scan/engineering/technology/txt\\_accordion1.html](https://www.nasa.gov/directorates/heo/scan/engineering/technology/txt_accordion1.html).



at a molecular and sub-molecular level are essential to advancements in this area. Thoughtful, strategically aligned equipment renewal plans are in place to assure this continued capability.

The Functional Polymers Group is to be commended for its strategic planning and identification of targeted growth directions in the following five areas:

- Molecules as Measurements,
- Composites for Infrastructure,
- Advanced Dental Composites,
- Advanced Chemical Separations in the Circular Economy, and
- Impact Behavior and Mechanics.

These areas are in alignment with the mission of NIST and many industrial corporate strategies.

The Polymers Processing Group is unique in that they have the scientific and technical expertise to perform very sophisticated and quantitative materials measurements during industrial processing of polymers. Good examples include neutron imaging in a running polymer extruder head, as well as numerous simultaneous scattering and spectroscopy techniques to study the development of crystallinity of polymers during processing. In most institutions, crystallinity is measured as a single end result number from processing, as opposed to NIST's approach of deeply understanding this extremely important time-based mechanistic phenomenon that results in final polymer properties. This theme of in situ measurement and understanding, which is also evident in other groups within MSED, is essential to enable the next generation of manufacturing in the United States and the world (Industry 4.0 approach). Having quantitative, accurate, in situ measurements enables active, closed-loop process control. This results in more statistically reliable polymer components and a wider application of polymers in society. The Polymers Processing Group is also to be commended for its technology transfer accomplishments, such as the Rheo-Raman-Microscope with ThermoFisher Scientific, TA Instruments, and Anton Paar.

The Functional Nanostructured Materials Group has unique capabilities in synthesis (e.g., materials foundry with capabilities in thin-film deposition, crystal growth, and 2D materials and nanoparticle synthesis), characterization (e.g., suite of magnetic measurements, spectroscopy, electrical measurements, and microscopy) and modeling (e.g., multiscale and machine learning). Its suite of tools for magnetic measurements coupled with modeling and synthesis capabilities define the group. The Functional Nanostructured Materials Group gave three presentations on specific projects, namely Electrochemical Processes, Metrology of Magnetic Materials, and Low Dimensional Electronic Materials. The Electrochemical Processes project team continued work on understanding the electrochemistry of the filling of recessed surface features for building complex structures, which was impressive particularly as it fills a well-defined industrial need. The group developed a new process for bottom-up gold-filling of recessed structures and gained a mechanistic understanding of the process and transitioned the technology from laboratory to manufacturing. In the Metrology of Magnetic Materials effort, there was a transition of the magnetic thin-films device effort to low-D materials project as the former aligns better with the electronics/quantum application space of the low-D project. The stated objectives are very well-aligned with NIST's missions for development of new measurement methods and instrumentation for characterizing 0D, 1D, 2D and 3D materials and development of new magnetic standard reference materials (SRMs). Much of the efforts in this area are a work in progress. The Low-dimensional Electronic Materials and Magnetic Thin Films team's goals were to develop libraries and advance metrology of 2D materials and quantum materials. The single-crystal growth facilities are good and include Bridgeman growth, chemical vapor transport, and CVD (crystal vapor deposition) capabilities. The magnetic engineering research facility (MERF) was excellent with coupled synthesis, processing, and novel advanced characterization capabilities. The team is developing advanced imaging and metrology techniques for characterization of spintronic materials and devices. Such expertise, capabilities, and resources are important to the development of emerging electronic and magnetic materials.

## **Opportunities and Challenges**

There is a need for comprehensive strategic planning to define clearly and outline the envisioned trajectory for MSED scientifically, given the limitations on resources. Such planning would consider the number of scientific staff and specific scientific expertise needed, equipment development needs, standards development needs, and prioritize all needed investments. Ideally, the strategic planning might include a shorter-term and a longer-term horizon. Having a well-developed plan that is clearly articulated to MML leadership will go a long way toward obtaining support.

**RECOMMENDATION 5-2:** The Materials Science and Engineering Division should develop a clear articulation of a broad-based strategic plan of the division and state how that plan reflects the overarching strategic plan of the Material Measurement Laboratory.

## **PORTFOLIO OF SCIENTIFIC EXPERTISE**

### **Accomplishments**

The quality of the NIST scientists and technical staff is very high as is their commitment to the organization. The technical team has the expertise required to accomplish programmatic objectives.

### **Opportunities and Challenges**

However, as indicated above it would be helpful to link to a fuller divisional plan to aid in assessing the scientific portfolio. Additionally it was pointed out that often NIST's unique and specialized expertise disappears with the retirement of key personnel.

## **ADEQUACY OF FACILITIES, EQUIPMENT, AND HUMAN RESOURCES**

### **Accomplishments**

The equipment and facilities for the work reported was very good to excellent particularly with regard to data quality. Some equipment needs updating, which might best be handled through a thoughtful, strategic equipment renewal process. The division staff has communicated a long list of big-ticket items in terms of equipment that will be needed. These need to be carefully evaluated in a comprehensive strategic plan, together with a prioritization of equipment needs. These processes will need to emphasize "unique" equipment needed to further measurement science, standards and technology, even in areas such as electron microscopy to differentiate NIST from other federal laboratories.

There is clearly a positive culture where permanent staff, postdocs, and visiting researchers feel valued and are proud of their work. This culture translates into almost all postdocs desiring to stay at NIST if that opportunity was available. Postdocs expressed that a positive culture existed for female and minority students.

### **Opportunities and Challenges**

In this era of constrained budgets, it will be necessary to prioritize equipment needs as well as take a survey of building infrastructure. From the overall division presentation, it was apparent that there is significant frustration with the laboratory operational model. An across-the-board 50 percent tax on all

equipment purchases heightens the trade-off between such purchases versus additional staff. For any equipment that is expensive (\$1 million to \$2 million or more), this effect can be substantial. Such a tax does not exist for large-equipment purchases in many universities, laboratories, or corporations. Second, the NIST working capital fund model for purchase of new equipment requires payback for any purchase from annual operating funds (that is, the funds that would otherwise go to pay staff salaries). Other agencies (such as the National Oceanic and Atmospheric Administration, the Department of Energy, the National Institutes of Health, and the Department of Defense, etc.) place a line item for expensive equipment in their annual budget request and treat equipment funds as separate from operating funds.

The support infrastructure (e.g., buildings) for the staff and equipment needs review and improvement. Although equipment and staff are appropriately prioritized over buildings, there have been instances where failures of the infrastructure compromised equipment with resulting impact on mission delivery. As an example, one laboratory flooded, resulting in damage and equipment downtime.

**RECOMMENDATION 5-3:** The Material Measurement Laboratory (MML) should evaluate how it budgets new equipment purchases and how this figures in to the resource management in its divisions. The MML should further remain aware of the damage to equipment due to flooding and other problems with buildings and facilities.

The hiring of term-hires (e.g., postdocs) as opposed to permanent hires is an issue. While the permanent hires are often preferred, personnel-related issues such as overhead and so forth appear to have prevented hiring of the latter type.

Mentoring and career planning of postdocs appears somewhat ad hoc with many postdocs expressing “opaqueness” about their career options. It was noted that early stage “beta” testing of a limited mentoring program is under way.

Finally, although diversity and inclusion was a difficult topic to assess in the time permitted, additional work in this area would better establish concrete programs and review processes to assure continued success.

## DISSEMINATION OF OUTPUTS

### Accomplishments

MSED is addressing stakeholder needs, especially at the higher TRLs. In addition, there was adequate monitoring of stakeholder use and impact of program output. It was noted that there was good dissemination of results using print media (high-impact journals).

### Opportunities and Challenges

Results from primary work in MML could be highlighted more. This could be accomplished using forms of media such as YouTube. In addition, a review of the effectiveness of the NIST website in communicating specific examples of unique and transformative contributions to the nation likewise could be beneficial.

In general, many federal laboratories are criticized for their scientific metrics. Typically, a good scientific metric for a full-time scientist will be 4-5 papers in leading journals per year. While this may be true in academia where the focus is on publications, at federal laboratories such as NIST, other mission-related impacts need to be prominently articulated and disseminated, such as critical and transformative advances in measurement science, standards, and technology.

**RECOMMENDATION 5-4:** The Material Measurement Laboratory should increase its activities aimed at communicating its accomplishments to its customers, collaborators, and audiences. This should include greater effort at highlighting results from the primary work of the laboratory. This could be accomplished using forms of media such as YouTube and improving the effectiveness of the NIST website by adding specific examples of unique and transformative contributions.

## 6

**Materials Measurement Science Division****INTRODUCTION**

The mission of the Materials Measurement Science Division (MMSD) is to ensure and promote excellence in measurement science. MMSD conducts mission-based fundamental research, standards production, and applied science and engineering. MMSD provides measurements for the determination of structure, composition, and properties of materials. Its Standard Reference Materials (SRMs) and Standard Reference Data (SRD) are used to validate methods and to enable new technologies. MMSD provides state-of-the-art instrumentation, methods, models, and software to measure materials over a range of length and time scales. MMSD projects and programs are well aligned with the mission of the NIST Material Measurement Laboratory (MML).<sup>1</sup>

MMSD has five major technical program areas. These programs are centered around core competencies that represent the expertise of the division. Each program consists of multiple projects and most are designed to be intra-divisional collaborations. The five program areas are (1) Atomic Arrangements and Structure–Property Relationships, (2) Physical Chemical and Mechanical Properties of Materials, (3) X-Ray Scattering and Spectroscopy, (4) Materials and Metrology for Safety, Security and Forensics, and (5) Informatics and Artificial Intelligence for Materials Design. MMSD conducts research to enhance its core capabilities and to promote innovation. The division has a balance between basic research, which is published in peer-reviewed journals, and technical projects that serve the standards and regulatory mission of NIST and requests from other stakeholders.

MMSD currently has 99 federal employees and 51 associates (contractors and guest scientists), making it one of the larger divisions. The majority of MMSD personnel are located at the NIST main campus in Gaithersburg, Maryland, where they are distributed primarily across three campus buildings. Six of the federal employees and four of the associates that are part of MMSD are located at the National Synchrotron Light Source II facility (NSLS-II) at Brookhaven National Laboratory in Upton, New York. From a funding perspective, MMSD receives 25 percent of its support from seven U.S. government agencies outside of the Department of Commerce.<sup>2</sup> These external collaborations are an important mode of dissemination of expertise and technology.

Three areas targeted for future growth are (1) ceramic additive manufacturing, (2) producing high-quality, machine-readable data sets, and (3) autonomous experimentation.

MMSD is organized into nine organizational units—the division office and eight technical groups based on technical expertise, but collaborations across groups are commonplace.

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<sup>1</sup> R. David Holbrook, 2020, National Institute of Standards and Technology (NIST), “Materials Measurement Science Division: NASEM Panel Review,” presentation to the panel, September 9.

<sup>2</sup> Ibid.

## ASSESSMENT OF TECHNICAL PROGRAMS

A brief assessment of the technical work is presented below. The discussion is organized around each of the eight technical groups in MMSD.

### Accomplishments

The Nanomechanical Properties Group (643.09) develops nano-scale measurement metrology and manages a laboratory dedicated to nanomechanics. Work includes equipment development and the calibration and control of mechanical properties. Measurements are performed at small scales and on small-scale phenomena. Property measurements include elastic modulus, plastic yield stress and fracture toughness, strength measurement, and strain and stress measurements. This group develops reference materials and measurement protocols for a number of both static and dynamic nanoproperty techniques, including high-resolution electron backscatter diffraction and scanning probe microscopy.

The Materials Structure and Data Group (643.08) develops and broadly disseminates measurement science, standards, and technology for the determination of the structure of advanced materials across a broad range of length scales. The group uses and develops in-house characterization tools and extensively exploits national user facilities for both synchrotron X-ray and neutron scattering. The group members determine, compile, evaluate, and disseminate key data and computational tools needed to establish the relationships between structures and performance of inorganic and hybrid materials and devices. One project includes developing machine-readable crystallographic descriptions to translate symbolic data into a format suitable for artificial intelligence (AI) applications. New projects have been initiated in development of 4D scanning transmission electron microscopy (4D STEM) electron diffraction, additive manufacturing, and advanced gas sorbent materials.

The Synchrotron Science Group (643.06) develops and disseminates state-of-the-art synchrotron X-ray measurement science, standards, and technology for the determination of the structure of advanced materials. Located at the NSLS-II, the group develops and maintains three high-throughput beamlines that provide timely access to X-ray facilities to support NIST priority programs. It also supports the broader scientific community as part of the NSLS-II General User Program. It is currently developing two resonant soft X-ray microscopy beamlines.

The Microscopy and Microanalysis Research Group (643.02) “performs fundamental research and develops metrology towards the compositional and morphological characterization of materials from the mesoscale to the atomic scale using electron, ion, and photon interactions with matter.”<sup>3</sup> The group determines composition and structure of nanomaterials and conducts comprehensive analysis, modeling, and theoretical methods to support stakeholder needs to advance microanalysis in diverse areas of materials, biological, and forensic sciences. They further maintain a microscopy facility.

The Nanomaterials Research Group (643.03) develops metrology to advance nanomaterials research and applications in emerging areas (e.g., nanomedicine, nanotherapeutics, nanoplastics). Measurement science is used to determine physical and chemical properties of materials in the nanoscale regime. The group develops physical and/or documentary standards related to nanomaterials, particle sizing, and surface analysis.

The Materials for Energy and Sustainable Development Group (643.04) “develops and disseminates measurement science, measurement standards, and measurement technology that pertains to the measurement of functional properties of advanced energy related materials.”<sup>4</sup> This work encompasses chemical, electrical, thermal, and magnetic properties, materials efficiency, and critical materials. New

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<sup>3</sup> Keana Scott, Group Leader, NIST, 2020, “Microscopy & Microanalysis Group: 643.02,” presentation to the panel, September 10.

<sup>4</sup> NIST Material Measurement Laboratory (MML), 2020, “National Academies of Sciences, Engineering, and Medicine: 2020 Assessment Read-Ahead Materials for September 9-11, 2020,” Gaithersburg, MD, p. 78.

themes include sustainability and the circular economy, the materials data infrastructure, and innovations in AI.

The Surface and Trace Chemical Analysis Group (643.05) develops, improves, and standardizes analytical techniques used for the elemental, molecular, isotopic, radiological, and morphological characterization of surfaces, thin films, and particles. The group also develops novel methods of chemical analysis based on optical microscopy, mass spectrometry, chromatography, ion mobility spectrometry, optical spectroscopy, autoradiography, and nuclear counting techniques. This group supports the NIST mission in safety, security and forensics.

The Security Technologies Group (643.10) conducts research to advance and develop the measurement science for trauma-mitigating materials and materials systems to identify concealed threats and contraband and to support the development of performance-based standards in the same area. Further, this group performs research on fundamental structure, properties, and performance to support innovation and advanced manufacturing of high-strength textiles, nanocomposites, and blunt-trauma-reducing materials.

### Challenges and Opportunities

The members of MMSD are extremely capable and productive in the broad area of materials measurement science. Their work is well aligned to the mission of NIST. The technical programs represent a balance of high-end research in measurement science and technology and support of commerce through stakeholder engagement. Research focus on nanoscale measurements and materials is providing exciting new knowledge of materials and enabling new avenues for materials fabrication, characterization, synthesis, and applications.

The new effort focusing on separation, characterization, and quantification of soft materials has progressed well and is an area for growth. Likewise, the success of the Nanomedicine Collaboratory points the way to additional collaborations.

**FINDING:** The development, fabrication, and sale of SRMs and documentary standards are central to the mission of MMSD. Although MMSD has a broad client base for SRMs, etc., the contacts are handled by other groups in the MML.

**RECOMMENDATION 6-1:** The Materials Measurement Science Division (MMSD) should increase the degree to which it utilizes its customers for feedback on new products and information with regard to emerging opportunities. To this end, the Material Measurement Laboratory should utilize a process for obtaining feedback. MMSD should increase its interaction with the offices managing sales of such products at NIST.

**FINDING:** In 2017, MMSD initiated a new effort focusing on the separation, characterization, and quantification of nanoscale soft materials (including plastics) by adopting previously developed methods and by investigating new approaches.

**FINDING:** The shift in emphasis toward nanoscale soft materials is an excellent area for growth but may require new equipment and expertise, because the group was previously focused primarily on hard materials.

**FINDING:** The group name for the Materials for Energy and Sustainable Development Group seems to be outdated. While there is research on energy materials, the increasing focus of the group appears to be in the area of high-throughput materials, materials data, and autonomous materials science.

**RECOMMENDATION 6-2:** The Materials Measurement Science Division should evaluate whether to move some of the work of the Materials for Energy and Sustainable Development group (e.g., X-ray Metrology) to another group (e.g., Materials Structure and Data Group) and refocus the former group's efforts on materials data and artificial intelligence approaches.

The Security Technologies Group still appears to be a bit of an outlier in the division, but clearly progress has been made to engage the work of the group into a cross-cutting research program that includes the following: (1) Atomic Arrangements and Structure–Property Relationships, (2) Physical Chemical and Mechanical Properties of Materials, and (3) Materials and Metrology for Safety, Security, and Forensics. There are additional opportunities for the Security Technologies Group to better exploit the extensive materials characterization capabilities of the other groups in the division.

## PORTFOLIO OF SCIENTIFIC EXPERTISE

### Accomplishments

At the time of the panel's review, MMSD staff consists of 87 scientists, 1 NIST fellow, 3 technicians, 2 administrative personnel, 6 support personnel, and 51 associates.

The Nanomechanical Properties Group core expertise includes the application of techniques to explore materials properties at the nanoscale. Techniques include scanning probe microscopy, nanoscale force spectroscopy, colloidal probe force spectroscopy for strength measurements, high (angular) resolution electron back-scattered diffraction, contact resonance AFM (atomic force microscopy), Raman microscopy, cathodoluminescence spectroscopy, X-ray diffraction, fluorescence spectroscopy, and coherent gradient sensing interferometry for accurate strain and stress measurements.

The Material Structure and Data Group members are experts in all major techniques of structural analysis—various modes of X-ray/neutron scattering, X-ray absorption spectroscopy, impedance spectroscopy EPR (electron paramagnetic resonance), EXAFS (extended X-ray absorption fine structure, TEM (Transmission electron microscopes), 4D-STEM, EELS (electron energy-loss spectroscopy), XEDS (Energy-dispersive X-ray Spectroscopy), and modeling.

The NSLS-II National User Facility reached full operation in November 2019. The X-ray beamlines probe the structural, chemical, and electronic properties of a wide range of materials. The facility features seven experimental stations and two unique dual beam stations. Measurements include near edge X-ray absorption fine structure (NEXAFS), hard X-ray photoelectron spectroscopy (HAXPES), and resonant soft X-ray scattering (RSOXS) with a novel data collection/analysis capability. Techniques are applicable to the new thrust in soft materials and, more generally, provides capabilities that are accessed by a broader user group.

The Microscopy and Microanalysis Research Group has expertise in a wide range of microscopy methods for application in compositional and morphological characterization of materials from the atomic to the mesoscale. Advanced measurement methodologies are achieved through expertise in maintaining, modifying, enhancing, and building state-of-the-art facilities.

The Nano Materials Research Group has expertise in a diverse array of techniques and specializations, including particle sizing, nanomaterials and organic ligand synthesis, surface chemical analysis, soft materials, atmospheric aerosols and microparticle analysis, and applications and growth of nanocrystals and nanowires. Skills are being applied to develop metrology to advance nanomaterials research and applications. Examples are metrology for soft nanomaterials and the link between structure and properties at the nanoscale.

The Materials for Energy and Sustainable Development Group has expertise in energy conversion materials and techniques, high-throughput experimentation, recycling and sustainability, X-ray metrology and standards, materials data, and autonomous materials science.



The Surface and Trace Chemical Analysis Group has expertise across a wide range of techniques applicable to measurement, technique development, materials handling, and standards creation for the characterization of particles, surfaces, and thin films. This expertise in metrology finds applications in safety, security, and forensics, including trace contraband detection and worker safety.

The Security Technologies Group has expertise in metrologies for property determination of high-performance materials and the advancement of technologies applied to security imaging. Performance-based standards are built on new technologies and knowledge of materials properties and structure.

**FINDING:** The Security Technology Group differs from other groups in MMSD in that its work has a significant focus on current “real-world” issues. Its members recognize the need to target those areas that are most urgent and on changes that can be readily adopted.

### **Challenges and Opportunities**

MMSD staff is excellent and taking good advantage of the unique research environment at NIST to conduct long-term research using state-of-the-art facilities, with talented co-workers, and a wide range of outputs for successful work. One of the staff stated that “impact” is a key metric for measuring output. As such, scientists will need to embrace that metric and measure themselves against it each year. Intra-division collaborations, shared resources, informal assistance, and exchange of ideas is essential to avoid silos and continuity of success. Continued attention will be needed to achieve a culture of sharing, assistance, and collaboration.

**RECOMMENDATION 6-3:** The Materials Measurement Science Division should conduct additional intra-divisional collaboration, which might be exploited to add fundamental understanding for the benefit of the research component of the work going forward.

## **ADEQUACY OF FACILITIES, EQUIPMENT, AND HUMAN RESOURCES**

### **Accomplishments: Human Resources**

Postdoctoral fellows are an important and significant part of the MMSD workforce that benefits both their scientific career and the MML. MMSD has begun both informal and formal mentorship for postdoctoral fellows. This includes an informal “on-boarding” interview with the division director to discuss NIST culture, projects, and current career plans. Mentorship is continual during the postdocs time at NIST. All mentors understand the importance of publication of work in reputable scientific journals. Attending scientific meetings is encouraged. Significant institutional support networks are available at NIST and external coursework is encouraged. Assistance with preparing for the time when their tenure at NIST ends is also provided. A debriefing interview includes feedback on how the postdoctoral program might be improved. A NIST postdoctoral fellowship can be a valuable career enhancing experience for the postdoc. Postdocs who go on to careers in university, industry, and so on, are one of MMSD’s successful products.

The NIST Summer Undergraduate Research Fellowship (SURF) Program, which sponsors an 11-week summer internship program for undergraduates, provides students with a hands-on research experience. This program was canceled for 2020 due to the global pandemic, and the number of students in 2019 was reduced due to the federal government shutdown. Otherwise, a typical number of students sponsored by MMSD each summer is 16, which is a good number. The support of the scientific staff enables the success of this program.

## Challenges and Opportunities: Human Resources

MMSD, as noted before, has 99 federal employees and 51 associates, a decrease from 106 and 85, respectively, from 2017. The major area of decline noted is with the associates, which decreased from 85 in 2017 to 51 at present. The decline in associates reflects the fact that several were hired full time. There was also a decrease in the number of postdoctoral researchers. The decline in the number of scientists in the past 3 years thus appears problematic, considering the need to maintain and grow expertise in critical areas. Further, several scientists are reaching retirement age.

As highlighted in previous assessment reports in 2014 and 2017, there is a dearth of technicians in the division, and a further reduction may need to be addressed. The reduction in the number of associates (primarily in groups 04, 05, 08, and 10) was said to result not in a lower number of work hours, but it was a transition from part-time to full-time associates. While it is not clear what the impact of this transition will be on the division, it may lead to associates taking on roles similar to career staff without the benefits of a permanent position.

**RECOMMENDATION 6-4:** The management of the Materials Measurement Science Division will need to continue to evaluate and understand the impact of the change in staff numbers and redistribution of workloads. Specifically, there needs to be a shared understanding of the division mission that justifies staff numbers.

MMSD needs continued focus on diversity of the scientific staff, as the division has the lowest percentage of female employees in MML. Addressing this problem at the entry level is necessary, perhaps not sufficient.

**FINDING:** The MMSD has the lowest female-to-male ratio compared with other divisions in the MML.

**RECOMMENDATION 6-5:** The Materials Measurement Science Division (MMSD) should examine ways to recruit and retain greater numbers of female scientific staff. MMSD staff should all work to enhance the visibility of NIST as a career option through technical meeting/society activities and university interactions. All team members should ensure inclusiveness and assist with career development of the diverse workforce, including the careers of associates and post docs.

Critical expertise that must be maintained needs to be identified, and action needs to be taken where expertise is at risk, such as with a single employee or an employee close to retirement. Another challenge for MMSD is recruiting new employees and working on employee retention. Recruitment needs to be early and “aggressive.” Research staff can seek opportunities to deliver lectures at universities in order to increase awareness of NIST and NIST career opportunities among the student population. The discussion of high-end research with a view to real-world applications will hold student’s attention. Participation by NIST’s diverse workforce will demonstrate a welcoming and inclusive work environment. Technical society activities also provide opportunities for student engagement.

Employees need opportunities to maintain and grow technical expertise, to interact with the external technical community through participation in technical meetings and workshops, and to be recognized as experts in their field. Also, high performers need to be recognized and be given opportunities for growth within NIST. External recognition of MMSD employees also brings recognition to NIST.

### **Accomplishments: Facilities/Equipment**

The work of MMSD is very equipment-intensive. Instrumentation is used for much of the in-house research. Further instrument improvements, invention of new instrumentation, and recommendations for use are part of enabling stakeholder best practices. NSLS-II is a tremendous national resource that is available to both NIST scientists (50 percent of the time) and the NSLS-II user community.

### **Challenges and Opportunities: Facilities/Equipment**

The division has developed a number of beamlines that are both a NIST and a national resource. Half of the beam time is open to general users and half to NIST users. This facility represents a large investment by NIST in developing synchrotron techniques over the past 20 years. One recent example is a new soft X-ray scattering facility built in part with an Innovations in Measurement Science award (\$1.5 million per year for 4 years). This is an exciting new capability. However, there is no clear funding for maintaining this new facility. Additionally, the group is working on two new X-ray microscope beamlines. The funding of this facility may be beyond the expectations of a division. Thus, a funding model at a higher level in the organization may need to be developed.

The project on developing Atom Probe Tomography faces a resource challenge. While this is a productive research area, the project uses a 3D atom probe instrument that is nearing 10 years in age and will need to be replaced or upgraded. This is just one of many important instrument needs of the division and might require better quantification of the impact of equipment development with respect to long-term maintenance.

Overall, the division is challenged by the need to refresh and replace state-of-the-art equipment. Given the current budget limits, this may not be possible for all equipment, and some tough choices will most likely need to be made. The division already extensively uses national user facilities for synchrotron and neutron measurements. This may have to extend to other techniques (e.g., electron microscopy) available at national user facilities for advanced characterization of materials. This cannot easily be done for research programs that are based on modifying, extending, and enhancing the capabilities of metrology equipment. Some effort may need to be made to centralize some equipment to the division level instead of the group level to remove any redundancy in equipment. Similarly, some programs may need to be eliminated if the base equipment becomes out of date and cannot be replaced.

The greatest need is driven by high-cost (>\$2 million) instrumentation and funding for facilities at NSLS-II. All equipment needs to be maintained and periodically refreshed. These issues are exacerbated by NIST policies and practices that add cost to purchases and that combine budgets for equipment and operations. Equipment-intensive experimental work relates directly to the NIST measurement science mission and needs to be addressed at the highest levels of NIST. Facilities such as the cleanroom in Building 218—with a low particle environment, temperature stability, humidity stability, and vibration isolation—are an example of the laboratory environment that is needed for certain instrumentation and sample preparation.

The purchasing power of the divisions is impacted first by a 50 percent tax on equipment. This disadvantages equipment purchases for the purposes of budgeting, because the trade-off—versus funding an additional staff position or other expenditures—becomes more acute. Further, the NIST working capital fund model for purchase of new equipment requires payback for any purchase from annual operating funds. This further disadvantages equipment purchases in any discussion of budgeting. Other agencies (such as the National Oceanic and Atmospheric Administration, the Department of Energy, the National Institutes of Health, and the Department of Defense, etc.) place an entry for expensive equipment in their annual budget request and treat equipment funds as separate from operating funds.

**FINDING:** MMSD recognizes the need for sustainable funding for higher-cost instrumentation (>\$2 million) as a division priority. The Synchrotron Science Group has recently developed beam lines at NSLS-II supported by division funds. NIST policies that add cost to purchases increases the burden. Other needs are to address aging buildings and facility requirements for special instrumentation. (See Recommendation 5-3.)

**FINDING:** The work of MMSD is extremely dependent on access to state-of-the-art instrumentation. New technologies are needed as a group moves into exciting new areas such as soft materials. Other instrumentation is aging and will need replacement in the near future (e.g., 3D atom probe instrumentation and electron microscopes). NIST extensively uses national user facilities beyond MMSD, particularly when instrument development is not a part of the project.

**RECOMMENDATION 6-6:** The Materials Measurement Science Division should prioritize the division's needs for upgrading/replacement of equipment and explore centralizing commonly used instrumentation at the division or laboratory level.

## DISSEMINATION OF OUTPUTS

### Accomplishments

Briefing and background materials presented to the panel showed many noteworthy examples of recognized outputs, such as publications (409 in archival journals, 22 conference papers, 114 NIST reports, and 1 book or book chapter), customer engagement (19 workshops, 8 CRADAs (Cooperative Research and Development Agreements), 2 MTAs (Material Transfer Agreements), 2 NDAs (Non-Disclosure Agreements), and 18 IAAs (Inter/Intra-Agency Agreements), standards activities (68 SRMs/RMs, 60 standards committees, and 15 leadership positions), patent and invention disclosures, external recognition, and Department of Commerce and NIST named awards.

MMSD has a clear customer focus. Partnerships with outside organizations account for 25 percent of the MMSD annual budget. These partnerships are with government agencies such as the Department of Homeland Security, the Department of Defense, the Department of Justice, the Consumer Products Safety Commission, and national laboratories. External partnerships also include universities and industry. These partnerships are a mechanism for dissemination of materials and know-how as well as a source of expertise and knowledge for NIST.

During the review period, the number of publications ranged from 151 to 174 peer-reviewed publications. The number of citations for the papers published in 2017 is 1,300, indicating that the papers are being well cited.

MMSD makes a tremendous contribution to the development of SRMs and standards, which are in demand by outside organizations. One example is RM 8012 and 8013 Gold Nanoparticles released in direct response to a request from the National Cancer Institute. The publication of physical and documentary standards is an important output of the division. Examples include "A Standard test Method for Estimating Limits of Detection in Trace Detectors for Explosives and Drugs of Interest" and "Standard Practice for Soft Armor Conditioning by Tumbling." MMSD scientists serve on standards development committees in a technical capacity both as leaders and as technical content contributors. Members of MMSD also serve in external leadership roles as journal editors, society directorships, and as members and chairs of steering committees. MMSD members have been elected to "fellow" status in a number of scientific societies.

## **Challenges and Opportunities**

One challenge for MMSD is maintaining the availability of a large number of SRMs over a long period of time, while at the same time developing new SRMs. Increasing public awareness of NIST activities, disseminating educational and instructional information, including tutorials, etc., can be used to increase impact. An example is the recent visualization of mask effectiveness in limiting the spread of COVID-19. The division might profitably expand collaboration with the NIST public affairs office.

Within the division, there are a number of examples where new code has been developed to analyze and process experimental data (e.g., OCEAN, RMC Profile, JARVIS, etc.). While this is an impact product that engages the broader materials community, it is difficult to quantify the impact of these codes. One way to quantify such impacts may be to request that the codes be cited in publications with a standard citation, allowing the impact to be tracked. Similarly, a major output of NIST is the development of new measurement capabilities. Again, MMSD will need to track and quantify the adoption of these new approaches in the broader community.

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**Biosystems and Biomaterials Division****INTRODUCTION**

The mission of the Material Measurement Laboratory’s (MML’s) Biosystems and Biomaterials Division (BBD) is “to promote U.S. biosciences and biotechnology innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life.”<sup>1</sup> BBD is currently focused on four primary areas—engineering biology, advanced therapies, precision medicine, and microbiome—with a drive to “foster innovation and build confidence in quantitative biology and biomaterial measurements across government and industry in support of the bio-economy.”<sup>2</sup> Importantly, in response to the COVID-19 pandemic, BBD implemented targeted initiatives by redirecting resources in manpower, collaborations, and equipment.

BBD has five groups—Complex Microbial Systems, Biomarker and Genomic Sciences, Biomaterials, Cell Systems Science, and Cellular Engineering—that are led by group leaders; scientists and an office manager report to each group leader. These cross-functional groups of scientists with expertise in materials, molecular biology, engineering, chemistry, microbiology, statistics, and data management are working well together. The BBD team is one of the world’s best technical teams, if not the best, in the development of advanced standards and innovative measurement technology to address the quantitative metrology needs of biological materials and processes.

In July 2020, BBD had 61 staff members and 24 associates, which represents 10 percent of the MML. The current staff number is an increase from 51 staff members and a decrease from 49 associates in 2017, the latter due to transfer of the collaboration with the American Dental Association Foundation to MSED. One member of BBD’s team has been named a NIST fellow, which is a very high honor and recognition of scientific excellence.

The 2020 budget is approximately \$21 million of which approximately \$18 million is from the Scientific and Technical Research Services (STRS) funds (an appropriation account), \$2.2 million is Other Agency (OA) Agreements, and \$0.7 million is Measurement Services. The budget has increased since 2017 (\$15 million) with the predominant increase derived from STRS targeted to engineering biology and regenerative medicine measurement standards.

BBD’s primary products are measurement science and protocols, which are disseminated in publications, reference materials, and reference data. Products include, for example, Genome in a Bottle<sup>3</sup> (GIAB) DNA, Cancer Biomarker EGFR (Epidermal Growth Factor Receptor) and MET, mixed pathogen DNA, Lentiviral vector, reference materials for flow cytometry and imaging measurement, advanced

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<sup>1</sup> Sheng Lin-Gibson, National Institute of Standards and Technology (NIST), 2020, “BBD Overview 2020 NASEM,” presentation to the panel, September 9.

<sup>2</sup> Ibid.

<sup>3</sup> “The Genome in a Bottle Consortium is a public-private-academic consortium hosted by NIST to develop the technical infrastructure (reference standards, reference methods, and reference data) to enable translation of whole human genome sequencing to clinical practice and innovations in technologies.” For further information, see NIST, “Genome in a Bottle,” <https://www.nist.gov/programs-projects/genome-bottle>, accessed April 26, 2021.

living reference materials (e.g., cancer and normal cells, Jurkat cells, genetically tagged yeast, microbial whole cell, human gut microbiome materials), validation of methodology, and international biological lexicon standardization.

## ASSESSMENT OF TECHNICAL PROGRAMS

### Accomplishments

BBD is currently divided into five groups, although the fluidity and rapid pace in what are termed focus areas often blurs the lines between groups. The stated focus areas are engineering biology, advanced therapies, precision medicine, and microbiome. Accomplishments were many and overall clear even if, in some cases, assignment to a particular group was not. Accomplishments across the division's groups include hosting of four consortia, organization of several dozen workshops, and leading or participating in nearly two dozen global standards development organizations. Consortia are flagship efforts involving companies, among many other stakeholders, and require investments of the division. Consortia have been organized in a topic once a critical mass of roughly five expert personnel in the division is achieved and when there is a perceived long-term and sustainable need for standards, especially for industry. NIST's Genome in a Bottle Consortium seems to be more than several years old and is maintained as an important accomplishment. The other three consortia were more recently created—in genome editing, quantitative flow cytometry, and rapid testing for microbial contaminants. Additional accomplishments beyond consortia over the past few years also include in excess of 130 journal publications, more than 10 ISO (International Organization for Standards) standards published, and multiple awarded patents. It is also an important accomplishment for BBD to have close coordination with the Food and Drug Administration (FDA), which is responsible for key approvals across focus areas of the division such as advanced therapies. One provided example is that NIST chairs ISO's Biotechnology Analytical Methods working group.

The Complex Microbial Systems Group advances measurements and standards for the exploitation of microbes. The group employs genomic, metagenomics, biochemical, and biophysical approaches to improve measurements on microbiomes, and it is also developing reference methods (RMs)—with attention to stability—on the sensitivity and specificity of pathogen-detection devices. Accomplishments include human gut microbiome (fecal) analysis standards to be used in a large multi-site international network, a microbial measurements standards workshop, microbe strain detection and identification within complex populations, and microfluidic development. Bacteria and yeast are the focus.

COVID-19, also caused by a microbe, shut down onsite work at NIST for months in 2020. Accomplishments by many across the division and NIST nonetheless began with remote work, including COVID-19 discovery-oriented analyses of protease function by meta-analyses and molecular simulations.<sup>4</sup> Upon restricted re-opening of laboratories, some groups are in the midst of contributing to useful standards, including for virus detection, which is finding application to sewage or wastewater. Expertise in flow-cytometry RM is being applied to antibody tests as a member of the National Cancer Institute's COVID serology network.

The Biomarker and Genomic Sciences Group develops measurement methods, standards, technology, and data for biomarker genomic sciences, including phenotype, and cell lines, including authentication, in order to support diagnostics and advanced therapeutics for cancer and other diseases. Flow cytometry calibration standards is one accomplishment that addresses multiple needs across a very large and growing community in academia and industry. Additional accomplishments include RM from

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<sup>4</sup> For further information regarding all of NIST's work related to COVID, see NIST, "NIST and COVID-19," updated March 30, 2021, <https://www.nist.gov/coronavirus>.

the Cancer Biomarkers Program computational resources for detection of different types of mutations or genomic variants as published in multiple papers in field-leading journal *Nature Biotechnology*.

The Biomaterials Group develops measurement capabilities and standards strategies to quantify biomaterials, biological systems (mammalian and microbial), and their interactions. Efforts extend to imaging and spectral methods and are important to biomanufacturing and translation of cell therapy and regenerative medicine products. Accomplishments include publication of a new theoretical basis for understanding population distributions and their fluctuations,<sup>5</sup> with a focus on iPS cells that many in academia and industry employ or plan to translate. The iPS work is done in close consultation with the Allen Institute of Cell Biology, which has parallel goals of quantitative cell biology and illustrates just one of the many strengths of the overall strategy.

The Cell Systems Science Group develops new measurements and models to elucidate complex biological phenomena at the cellular and subcellular levels. It establishes measurement capabilities, including bioimaging and other cytometry techniques, that examine attributes of cells, and develops measurement assurance strategies, including RMs. Accomplishments relevant to advanced therapy include development of an ISO cell counting standard and an ISO cell viability standard, which are generally relevant to dosage effects. In genome editing, which has expanded greatly in academia and industry with new methods over the past few years, the group has so far contributed to ISO lexicon, formed a large genome editing consortium with dozens of stakeholders, and leveraged NIST's GIAB RM for standards. Accomplishments in tissue engineering and in cell engineering, such as with Chimeric antigen receptor T cells (CAR T cells), include exploiting NIST's computational strength for artificial intelligence (AI) applications to pattern recognition. This led directly, for example, to a paper in the field-defining *Journal of Clinical Investigation*.

The Cellular Engineering Group is the newest of the five groups and combines state-of-the-art synthetic biology, automation of bench processes, and machine learning to generate living measurement systems, such as cells, that are engineered and standardized. Collaborators include the world-leading J. Craig Venter Institute as well as academic laboratories. Accomplishments include ISO standards in the area of genome synthesis and patents in the microfluidics realm relevant to synthetic cells.

## Challenges and Opportunities

COVID-19 testing and diagnostics are in urgent need of expertise that a well-networked and well-regarded BBD can in principle provide. The need and the efforts exemplify—as a key opportunity—the broader importance of quantitative life sciences research to the nation and to the world.

A challenge is the lack of dedicated resources for COVID-19 efforts. However, with suitable groups and expertise already in place, including recently developed efforts in lentivirus for cell therapy, BBD is pivoting resources to respond quickly to the pressing worldwide challenge. Serology testing is of great relevance to antibody responses and success in vaccine development, and BBD's expertise in standards-based quantitative flow cytometry assays is now the basis for active collaborations with the FDA, the National Cancer Institute of the National Institutes of Health, the World Health Organization, and various companies. This takes the form of services for standard control samples and also materials to validate tests. Diagnosis of virus in complex materials beyond nasal swabs include fecal material and wastewater as a rapidly emerging opportunity that can exploit BBD expertise in standardized and well-established GIAB material coupled to developing standardization of stable fecal material in earlier development. Although applied to COVID-19, applications are envisioned for other microbes that might range from annual influenza to bacterial contaminations and bio-threats.

Advanced therapy opportunities are emerging from many directions, including regenerative medicine, which is highly complex. BBD is well-poised to impact standards as well as discovery. Two of

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<sup>5</sup> J.B. Hubbard, M. Halter, S. Sarkar, and A.L. Plant, 2020, “The Role of Fluctuations in Determining Cellular Network Thermodynamics,” *PLoS ONE* 15(3): e0230076.



the four consortia illustrate the outside interest and the investment in flow cytometry and in rapid microbial testing methods. In the latter, there is a challenge to address the diversity of states of microbes, such as in biofilms that are certainly problematic in biomedical devices. Challenges in resources are incessant across the highly competitive realm of therapies. However, therapy-developing companies, such as AstraZeneca, are collaborating with BBD in standards-related research and innovative quality control measurements using the CRADA (cooperative research and development agreement) mechanism. Challenging overall with living systems and derived standards is the mutation rate in the DNA and other sources of variation, which require extra care about stability of averages and variances; but BBD is not only aware but also exploiting the opportunities provided by NIST's computational resources, such as in AI, to address some of the issues.

Biotechnology and engineering biology are perhaps less complex and more reductionist than above, providing clear opportunities for standards approaches. BBD is coordinating with other agencies, especially FDA. Laboratory automation combined with machine learning (ML) again exploits unique opportunities provided by NIST, including its resources in hardware and computation. Challenges are perhaps modest but real in integrating non-bio expertise such as automation engineers, chemists, and fluidics experts. Crossing boundaries in bio-discovery is nonetheless a credible opportunity for a multidisciplinary campus such as NIST, even though resource constraints are rightly viewed as a challenge.

Four consortia are flagship efforts with long-lasting opportunities involving NIST, companies, and many other stakeholders. As such, the ongoing challenge is to identify and matriculate into consortia those key efforts that can take off from multi-partner collaborations or networks.

## PORTFOLIO OF SCIENTIFIC EXPERTISE

### Accomplishments

BBD is a recognized leader in biometrology within the United States and internationally as demonstrated by BBD's standards development (measurement science and technology development) leadership in the BBD-led consortia—Genome in a Bottle Consortium, Mouse Cell-Line Authentication Consortium, Flow Cytometry Quantification Consortium, Genome Editing Consortium, and the newly established Rapid Microbial Testing Methods Consortium. Outcome products from these consortia are reference standards, innovative, reliable reference methods, benchmark sets, data, publications, NCBI (National Center for Biotechnology Information) database inputs, harmonized lexicon, and a repository of relevant microorganisms.

The scientific and technological expertise of BBD is excellent as evidenced by the numerous high-quality peer-reviewed publications (>130) in leading journals such as *Nature Biotechnology* and *Nature Methods*. Further, its scientific and technological leadership role in foundational measurement science and technology for complex biological systems is well supported by the fact that many of these publications are the products of collaborative studies with its consortia (66 in total) members.

Since the 2017 review,<sup>6</sup> groups in BBD have grown significantly in mammalian and microbial biologics scientific expertise and the groups have also increased in number by one, due to additional support for the Engineering and Biology and Regenerative Medicine initiatives. However, in spite of this scientific project expansion, the total budget of the division has not changed significantly due to (1) decreases in agency funds and (2) also decreases in the number of staff. The success of BBD in enhanced group activities appears to stem from efficient integration of staff among the groups and the use of modular and flexible capabilities. A good example of their efficient way of responding to challenges is the COVID-19 testing and diagnostics.

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<sup>6</sup> NIST Material Measurement Laboratory (MML), 2020, "National Academies of Sciences, Engineering, and Medicine: 2020 Assessment Read-Ahead Materials for September 9-11, 2020," Gaithersburg, MD.

BBD's work has been recognized by numerous awards to its staff externally, by the Department of Commerce (DOC) and NIST. Some noteworthy external award examples are the following: (1) C. William Hall Award by the Society of Biomaterials (2020), (2) Gears of Government Award by the U.S. government (2020), (3) two Presidential Early Career Awards for Scientists and Engineers (2017 and 2019), and (4) both an Outstanding Young Scientist and an Outstanding Young Engineer Award from the Maryland Academy of Sciences (2018 and 2019).

In some of the consortia, BBD's work is highly futuristic, as in the case of the human gut genome project. Uniquely, the human gut microbiome project has a very strong international presence.

### **Challenges and Opportunities**

Recognizing that complex biological systems are governed by the principles of thermodynamics, fluid mechanics, and colloidal science, BBD has some strength in these fields. Additionally, expanded expertise in virology, immunology, microbiology, and bioinformatics would benefit the BBD's mission. It is critical that this expertise be maintained and indeed strengthened further through new hires by BBD management and by interactions with other NIST divisions.

Since the 2017 review,<sup>7</sup> BBD has lost approximately 20 percent of its laboratory space. It has transitioned to an industry-like collaborative model where laboratories are designed by function, and space is designed to promote cross-team interaction. BBD has embarked on a multiyear laboratory and office space modernization plan.

BBD is responding to the ongoing pandemic and emerging biothreats by contributing to leading-edge measurements and standards. It lacks dedicated resources to sustain these efforts. To address the acute problems with COVID 19, BBD reassigned personnel from other necessary, but more long-term, projects. If standards work is to continue with corona viruses or other infectious disease vectors, this would be better handled with a dedicated set of scientists. However, the research and development (R&D) programs that BBD had developed prior to COVID-19 are vital to U.S. biologics manufacturing and research efforts. This implies that additional staff may be needed to continue both the existing programs and the recent work on coronavirus measurements and standards.

## **ADEQUACY OF FACILITIES, EQUIPMENT AND HUMAN RESOURCES**

### **Accomplishments**

BBD designed and built an adaptive, automated, AI-enabled modular unit, the Living Measurements Systems Foundry, which is providing quantitative measurement of complex living systems and processes as a key component of BBD's design-build-test-learn cycle to predictively engineer biological systems with the intent to accelerate R&D innovation and advance biomanufacturing. Notably, BBD has designed and installed a second modular unit, the Prototype Cell Assay Measurement Platform (P-CAMP), which is also adaptive, automated, and AI-enabled.

BBD has implemented state-of-the-art data sciences for data collection and analysis for imaging, cellular engineering predictive functional metrics, and quantitative assays to characterize CAR-T functionality/lentiviral infectivity. Additional research areas are in the queue for big data retention and analysis. New equipment for automated LN2 biologics storage, BioStore III, is in place. Referring to the 2017 review<sup>8</sup> recommendations, BBD's older chemical laboratories have been renovated to modern biological laboratories.

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<sup>7</sup> Ibid.

<sup>8</sup> Ibid.

BBD does not have a gender equality problem as its staff gender ratio (58 percent males, 42 percent females) is similar to that found in the field of biological sciences, which draws the interest of both females and males. The division chief is female as are two of the five group leaders. Of note, there is a broad age range within the scientific staff, which also allows diversity of thought and knowledge.

### **Challenges and Opportunities**

BBD has lost approximately 20 percent of its laboratory space, which negatively impacts program growth. Such growth could be accommodated by space in one of the new laboratory buildings envisaged in the NIST master plan for Gaithersburg,<sup>9</sup> while ensuring continued scientific interactions by addition of inside walkways that connect to existing NIST buildings.

Knowledge of complex biological systems is continually evolving with developing manufacturing methods and commercial biological materials. Interwoven knowledge in biology, chemistry, physics, math, and data and informatics is required. For BBD, this translates into a need for additional emphasis on colloidal science and thermodynamics, biofilm biochemists, and fluid mechanics.

It is unknown if underserved minority representation within BBD is reasonable or could be improved and is in need of assessment and elaboration of what steps, if any, need to be taken. At the corporate level, NIST has a working group to consider equity disparity that can further illuminate this issue.<sup>10</sup>

Postdoctoral fellows seem to be working at BBD for many years instead of moving forward with their careers (and out of postdoctoral positions). Setting term limits for postdoctoral fellows would be one way that BBD management could address this, along with promulgating a progressive plan for postdoctoral fellow placement in synergistic positions in industry, academia, or government.

## **DISSEMINATION OF OUTPUTS**

### **Accomplishments**

BBD has strong participation in national and international consortia, national and international working groups, and has a recognized international presence. BBD has published more than 130 peer reviewed articles in high-impact journals, been granted 3 U.S. patents, presented more than 280 invited talks and webinars, participated in numerous National Academies panels, provided standards expertise to State Department and regulatory agencies at international forums (Organisation for Economic Cooperation and Development, Asia-Pacific Economic Cooperation, and the International Organization for Standardization), and promoted commerce and trade by participation in global comparison studies.

BBD maintains more than 110 formal agreements—a very impressive number, organized 34 workshops, and led or participated in more than 20 global standards development organizations. Five NIST consortia—Genome in a Bottle, genome editing, quantitative flow cytometry, mouse cell-line authentication, and rapid microbial testing methods—have been hosted by BBD. BBD received the NIST Technology Maturation Acceleration Program Award in 2020 (\$250,000)—a key indicator. BBD is a member of and/or a leader of several working groups/policy forums such as the following: National Science and Technology Council’s (NSTC’s)<sup>11</sup> Biosciences Subcommittee and its Synthetic Biology Interagency Working Group and the Multi-agency Tissue Engineering Science Subcommittee (e.g.,

<sup>9</sup> For further information, see NIST, 2018, “Gaithersburg Campus Master Plan,” May, [https://www.nist.gov/system/files/documents/2018/06/15/nist\\_gaithersburg\\_master\\_plan\\_may\\_7\\_2018.pdf](https://www.nist.gov/system/files/documents/2018/06/15/nist_gaithersburg_master_plan_may_7_2018.pdf).

<sup>10</sup> NIST, 2019, “Inclusivity at NIST: Recent actions supporting equity in career advancement at NIST,” presentation to the Visiting Committee on Advanced Technology, October 24, Gaithersburg, MD.

<sup>11</sup> NSTC is an interagency strata of committees created by Executive Order. The Office of Science and Technology Policy is the secretariat.

FDA). BBD is also a member of NSTC's Committee on Homeland and National Security/Health Security Threat Subcommittee; chair of the ISO TC/276 Biotechnology Analytical Methods International Working Group and U.S. Mirror Technical Committee; a member of ASTM F04 Medical and Surgical Materials and Devices; and a member of American National Standards Institute.

BBD staff serve as the standards expert member in two manufacturing institutes—the National Institute for Innovation in Manufacturing Biopharmaceuticals (NIIMBL), which is DOC-funded to accelerate sustainable biopharmaceutical manufacturing innovation, and Biofabusa, which is Department of Defense-funded to make practical large-scale manufacturing of engineered tissues and tissue-related technologies. BBD helped to initiate and participates in the International Metagenomics and Microbiome Standards Alliance (IMMSA) whose function is to identify and disseminate microbiome measurements. BBD or its staff are members of the professional societies ISCT (International Society for Cell & Gene Therapy) and ISSCR (International Society for Stem Cell Research) as well as the accreditation bodies AABB and FACT (Foundation for the Accreditation of Cellular Therapy). Of note, the BBD director received the Gear of Government Award, and five other division members received prestigious awards.

### Challenges and Opportunities

Despite the plethora of outreach as demonstrated in the paragraph above, BBD has the opportunity to spread the word on its products and capabilities in industries, such as agriculture, that are not its traditional stakeholders or within small and medium enterprises. Additionally, while a challenge, resource uncertainty and erosion can lead to increased innovative opportunities with diversified resource pools.

**FINDING:** BBD has built an exceptionally strong network of collaborators and stakeholders comprised of government entities, academic institutions, and industry, which has allowed for strong technical programs and scientific capability. The challenge will be to continue to build these assets sustainably and further to enable agility as U.S. economic factors shift.

**RECOMMENDATION 7-1:** The Biosystems and Biomaterials Division (BBD) should (1) with creativity, develop a business strategy that focuses on BBD's unique products that may include licensing and further consortia for use of BBD products, services, and expertise; (2) strategically place BBD postdoctoral fellows into industry, academia, and other government positions to improve connectivity with outside current and future collaborators and stakeholders; (3) hire or contract with a communications person with YouTube and other media expertise to reach individuals who are searching for BBD-type expertise, products, and research services; and (4) determine how to connect with quality and manufacturing personnel at small and medium-sized companies in targeted industries. Emphasizing NIST BBD leadership, with thoughtfulness and quantification, in BBD program areas should be addressed by BBD leadership and staff to further enhance leadership with collaborators and stakeholders.

**RECOMMENDATION 7-2:** The Biosystems and Biomaterials Division should improve awareness of its products and capabilities, especially within small to medium-size enterprises and companies that are not currently stakeholders because they are in different industries (e.g., agriculture).

## OVERALL CONCLUSIONS AND RECOMMENDATIONS

A 20 percent reduction of BBD laboratory space has occurred, which impedes further growth of BBD project areas. The new laboratory buildings envisaged in the NIST master plan for Gaithersburg<sup>12</sup> would be beneficial and could be improved with the addition of physical connection (sky walks, for instance) to old NIST building(s) so that the benefits of interactions with other divisions are not lost.

Recognizing that complex biological systems are governed by the principles of thermodynamics, fluid mechanics, and colloidal science, BBD has maintained strength in these fields. However, it is critical that this expertise be maintained. Additional expertise in virology, immunology, microbiology, and bioinformatics would benefit the BBD mission. These scientific areas of expertise will need to be strengthened by BBD management further through new hires and by interactions with other divisions.

Continuity of staffing is a problem suffered by all entities, including BBD. BBD leadership might implement cross-training of staff with intent during each year to mitigate the effects of loss of key staff through retirement, illness, or job transition as well as strengthening scientific creativity by increasing each individual's knowledge.

There is a need to consider the career trajectory of postdoctoral fellows strategically. A logical strategy consistent with the MML mission would be to place postdoctoral fellows within current and potential stakeholders in order to enhance collaborations and cross fertilization of knowledge.

BBD is responding to the ongoing pandemic and emerging biothreats by contributing to leading edge measurements and standards. However, they lack dedicated resources to sustain these efforts.

**RECOMMENDATION 7-3:** The Material Measurement Laboratory should evaluate whether the square footage assigned the Biosystems and Biomaterials Division is commensurate with the division's current size and mission.

**RECOMMENDATION 7-4:** The Biosystems and Biomaterials Division should provide additional resources in thermodynamics, fluid mechanics, colloidal science, virology, immunology, microbiology, and bioinformatics in a manner commensurate with the increasing importance of these specialties.

**RECOMMENDATION 7-5:** The Biosystems and Biomaterials Division should analyze underserved minority representation among its staff and develop an action plan to address findings both from such study and from NIST's equity disparity studies.

**RECOMMENDATION 7-6:** The Biosystems and Biomaterials Division should develop a plan for outplacing long-tenured postdoctoral fellows into synergistic positions in industry, academia, or government. This plan should include an assessment of what shortfall, if any, this might create in its staffing plans.

**RECOMMENDATION 7-7:** The Biosystems and Biomaterials Division leadership should implement cross-training of staff with intent during each year to mitigate the effects of loss of key staff and ensure continuity.

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<sup>12</sup> For further information, see NIST, 2018, "Gaithersburg Campus Master Plan," May, [https://www.nist.gov/system/files/documents/2018/06/15/nist\\_gaithersburg\\_master\\_plan\\_may\\_7\\_2018.pdf](https://www.nist.gov/system/files/documents/2018/06/15/nist_gaithersburg_master_plan_may_7_2018.pdf).

## 8

**Biomolecular Measurement Division****INTRODUCTION**

The major focus of the Material Measurement Laboratory's (MML's) Biomolecular Measurement Division (BMD) is to develop measurement science, standards, and reference data for accurate and reproducible characterization of proteins, nucleic acids, glycans, metabolites, and lipids for use in biotechnology, DNA forensics, biomedical and bioscience research, and health care. The BMD has five groups that interact and cross fertilize their work, although in some instances cross-disciplinary interactions could be enhanced. They are as follows: Biomolecular Structure and Function; Mass Spectrometry Data Center; Applied Genetics; Bioprocess Measurement; and Bioanalytical Science.

The BMD main areas of research are in forensic genetics and illicit drugs, clinical diagnostics using protein and nucleic acid markers, mass spectrometry reference data and library, and advanced biotherapeutics, which include the biomanufacturing and the engineering biology programs. Core competencies are clearly at the cutting edge. Examples include the following: mass spectrometry (MS), liquid chromatography (LC), nuclear magnetic resonance (NMR), X-ray, neutron, and cryo-electron microscopy methods for determining biomolecular composition, structure, and amount; MS data analysis and building reference data products for chemical and biochemical identification; biophysical characterization of biologics and biological particle sizing; CE (capillary electrophoresis), digital polymerase chain reaction (dPCR), and NGS (next-generation sequencing) characterization of clinical and forensic genetic markers; development of protein, nucleic acid, and other biological reference methods (RMs); and cell culture/protein expression for R&D and development of RMs. The customers and stakeholders for BMD currently include four major research communities—clinical medicine, biopharmaceutical, forensic, and mass spectrometry. BMD has excellent partners in industry, federal government institutions, and laboratories. These include, but are not limited to, AstraZeneca, Novavax, the Food and Drug Administration (FDA), and NIH.

BMD currently consists of 81 staff members and 27 associates. BMD conducts research in two buildings on the main NIST campus and at the Institute for Biosciences and Biotechnology Research (IBBR) located on the University of Maryland, Shady Grove, campus in nearby Rockville, Maryland. BMD's operating budget for 2020 was \$32 million. IBBR is a joint institute between NIST's BMD and the University of Maryland Baltimore (UMB) and the University of Maryland, College Park (UMCP). Joint research activities with Maryland at IBBR are supported through a cooperative agreement of \$3.14 million from NIST to UMCP. A highlight of this collaboration since 2017 has been the establishment of cryo-EM measurement capabilities, which includes the installation of two new cryo-EMs at IBBR and a new sample preparation laboratory. The costs were shared by NIST, UMB, and UMCP.<sup>1</sup>

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<sup>1</sup> Michael Tarlov, NIST, 2020, "Biomolecular Measurement Division Overview: NASEM Panel Meeting," presentation to the panel, September 9.

## ASSESSMENT OF TECHNICAL PROGRAMS

BMD's scientific and technical portfolio is impressive, cutting across three areas—basic science and technology, stakeholder-driven research, and mission-based products. BMD is producing advanced and needed reference materials and standards that are addressing the current and pre-competitive markets in bioscience by providing high-impact products and processes with respect to reference materials and standard reference data (SRD). A few notable achievements resulting from the basic science and technology are the Next Generation Protein Sequencing (NIST phe/Trp NAAB), the Sub-Zero Chromatography System for HDX-MS, and the Deep Neural Networks to predict gas chromatography retention indexes.

### Accomplishments

BMD has continued to develop and apply formidable capabilities across a range of measurement science and tools. These include the following:

- NIST Mass Spectrometry Data Center and libraries;
- DNA forensics, which was recently leveraged for advancing and ensuring quality of nucleic acid-based testing for COVID-19;
- Biomolecular reference materials for applications in clinical diagnostics, food safety, and biopharmaceutical development and manufacturing;
- NIST's biomanufacturing program (as lead), resulting in reference standards for monoclonal antibodies (e.g., NISTmAb RM 8671), accurate measurement of protein aggregates in drug products (RM 8634), and a polymer-based reference material; and
- NISTCHO (CHO cells) as an open innovation platform for fostering fundamental understanding and development of mammalian cell lines employed in the manufacture of protein biotherapeutics.

### Analytical, Reference Materials (and Software), Research Capabilities

These analytical capabilities and reference materials have been developed under a well-defined structure led by the chief and deputy chief of the division. Within the division, the Biomolecular Structure and Function Group, located at the IBBR in Rockville, develops advanced biomolecular structure measurements relevant to the biopharmaceutical and biotechnology industries. The Mass Spectrometry Data Center Group “measures, compiles, evaluates and disseminates” standard reference data and analysis software for GC-MS (mass spectrometry) and LC (liquid chromatography)-MS, with current emphasis on proteomics, metabolomics, and forensics. The Applied Genetics Group leads in the development of standards and measurement technology for human identification and biometric law enforcement using genetic information. Bioprocess Measurements addresses measurement needs relevant to biological industrial processes including protein particles and novel sensors for health care. The U.S. requirements for determining composition, structure, quantity, and function of proteins, peptides, and metabolites are in part addressed by BMD's Bioanalytical Science group. Staffing for these capabilities, based on 108 people (total), includes 69 scientists (ZP), 4 technicians (ZT), 6 support staff (ZS), and 27 associates.

### Stakeholder Needs

BMD has addressed its stakeholder needs by developing the NIST20 Mass Spectrometry Libraries, the 2D-NMR for HOS of mAb therapeutics, and advancing NGS technology for human

identification. Finally, BMD has developed three outstanding mission-based products: NISTmAb8671 reference material, the RM8634 ethylene tetrafluoroethylene for particle sizing, and the SARS-CoV-2 research-grade test material. The latter product has assisted a number of companies in their development efforts for antibody test kits for COVID-19.

## **Budget**

In the budget for BMD, approximately one-third the funding is allocated to the MS Data Center, with the remaining budget being divided among the other four groups and division headquarters. Overall, these groups have shown significant accomplishments with the stated goals and the resources allocated. Accomplishments range from characterization of protein stability, protein structure, and production cell science, all of which are of significant interest to the biopharma industry. Concurrently, other accomplishments include methods for characterizing proteins from high order structure to biophysical characterization. Customer outreach through interlaboratory Measurement Comparisons, CRADAs (cooperative research and development agreements), and biopharmaceutical measurement roundtable are other examples of the effectiveness of BMD's work.

## **COVID**

BMD staff are applauded for their quick pivot to tackle the COVID-19 pandemic. The flexibility and creativity of their high-quality staff enabled a rapid re-orientation to provide COVID-19 RNA standards, form COVID-19 serology partnerships, e.g., with Lab Corp, initiation of COVID-19 spike protein MS library, and development of strategies to assess vaccine manufacturing quality and consistency.

## **Challenges and Opportunities**

### **Measurement Services**

BMD provides a range of measurement services of value to industry. This is exemplified by the services provided in forensics, in which the Applied Genetics Group of BMD shows exemplary cooperation, and impact with law enforcement agencies. Cooperation across BMD is encouraged and could be strengthened in some instances. The inherent challenge will be for management to encourage cooperation across various groups while obtaining additional resources when needed to carry out the additional work and for achieving longer-term diversity.

**FINDING:** There are opportunities for BMD to further serve the industry by continuing to develop its reference materials (structure analysis, standards, reference proteins, and living cells). The challenge will be to stay up to date with the latest industry developments and to amplify cross-disciplinary, cross-division, and interagency cooperation.

### **AI/ML Expertise**

The applications of artificial intelligence (AI) and machine learning (ML) have now permeated the science and engineering fields, enabling discoveries and insights not previously possible. Indeed, these methods have now become common and indispensable components of virtually all analytical or measurement methods. The list of BMD applications includes MS spectra/databases, NMR library



contours, retention index analyses, forensics, and others. An AI/ML expert would likely provide novel insights into the embedding of these methods throughout the division as well as playing an educational role.

**RECOMMENDATION 8-1:** The Biological Measurement Division (BMD) should evaluate its portfolio of expertise of staff with expertise in artificial intelligence and machine learning as applied to the measurement tools specifically in BMD. BMD might want to consider a joint hire with another division to leverage additional expertise and resources, or develop a more centralized collaboration model (i.e., community of practice) to make enhanced use of AI/ML expertise.

### **Non-Human Application Areas of Measurement Science**

The majority of BMD's application areas are human based, that is forensics, biotherapeutics, Chimeric antigen receptor T cells (CAR T cells), and so forth. Significant opportunities may be present in areas beyond that applied to humans; these include agriculture, veterinary science, biocatalysis, and environmental and marine research areas.

**RECOMMENDATION 8-2:** The Biological Measurement Division (BMD) should develop a strategy to assess agriculture, veterinary science, biocatalysis, and environmental and marine research areas as possible opportunities for growth and sources of additional collaborations and funding.

## **PORTFOLIO OF SCIENTIFIC EXPERTISE**

### **Accomplishments**

The quality of scientific expertise within the BMD represents the best that the MML has to offer. BMD has deep expertise in biomolecular technologies, including mass spectrometry, forensics, biopharmaceuticals, and NMR. Further extending the division's areas of expertise is the application of these and other methods to the measurement of a multitude of biologically important species: proteins, nucleic acids, sugars, lipids, and metabolites. The division has worked to grow its expertise in protein drug manufacture as well as cell-based drug production strategies via its work on CHO cells and CAR T cells. Additionally, the division possesses abilities that are among the best in the world for standards design, production, and distribution including NIST mAb (monoclonal antibody), NIST CHO (Chinese Hamster Ovary cells), protein aggregate standards and others. As an example, NIST mAb has been purchased and used by nearly all of top 20 global pharmaceutical companies, indicating the trust that the community places on BMD's scientific expertise.

BMD's staff are critical to the provision of high-quality reference materials, providing tools across the world that enable quality control, new instrument development, facile benchmarking, and comparison of results across platforms. BMD has also forged a high-value partnership with the University of Maryland through the aforementioned IBBR. This collaboration enables the BMD to access the deep knowledge base at the University of Maryland, adding to the available expertise. The expertise of the division is widely recognized both internally and externally. Internal recognition is evidenced by their many collaborations with other NIST divisions—for example, for AI/ML applications, protein sequencing efforts, and forensic partnerships. External expertise recognition is accorded by their broad collaborations with other governmental groups—for example, the National Institutes of Health, the Food and Drug Administration, Department of Justice, and many others.

## ADEQUACY OF FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

### Accomplishments

#### Facilities

The facilities for BMD are excellent and likely help to attract (and retain) the best and brightest scientists. The equipment and instruments are state of the art, and the transition from chemical sciences and standards research approximately 5 to 10 years ago to the new frontiers of bioprocess and biotherapeutic developments has been handled with amazing continuity between existing missions and future opportunities. This is a tribute to the leadership of BMD, but also presents challenges and opportunities, summarized below.

#### Human Resources

During the review, there were special discussion sessions stratified into early-, mid-, and late-career stage. This offered anecdotal insight into how these staff—including both full-time equivalents and associates—at all three stages were recruited and their talent developed. It appears that the MML attracts the absolute best and brightest postdoctoral employees. The NRC research associates (i.e., postdocs) hired by NIST<sup>2</sup> are on the cutting edge of research in their respective fields. The postdoctoral cadre is energetic, bright, and dynamic and a window to the future. The MML could capitalize on this, as well as develop the potential of these early-career people. The postdoctoral employees (i.e., associates and NRC postdocs) are mainly junior career and have noted that they would like better definition of pathways for achieving permanent status, or alternately assistance and mentoring for academic or industry careers outside of NIST, since only a fraction (30 percent) of postdoctoral or temporary employees achieve permanent status.

In discussions, mid-career staff expressed similar sentiments to the early-career researchers in that they sought a clear pathway to future career advancement—whether at NIST, academia, or industry. Bi- or tri-yearly reviews for mid-career staff is a procedure used in many European research institutions and has worked well to enable mid-career employees to move on. A clear goal that the mid-career employees seek is to become a NIST fellow. This was perceived to be out of reach or hard to obtain, absent mentors that would make the case for deserving people or areas and guide activities and priorities to achieve this status.

### Challenges and Opportunities

#### Facilities

There is an ongoing challenge in finding resources for maintaining existing infrastructure (leaky roofs, HVAC [heating, ventilation and cooling] in need of repair, etc.). Although equipment and staff are appropriately prioritized over buildings, there have been instances where failures of the infrastructure compromised equipment and had impact on mission delivery. The buildings on the main NIST campus may have exceeded their design life and are otherwise in need of repair. Finding resources to address this is difficult but critical to maintaining infrastructure that is consistent with, and will support operations of, exquisitely sensitive instruments and the brand for excellence that is associated with NIST worldwide.

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<sup>2</sup> “The NIST NRC Postdoctoral Program supports a nationwide competitive postdoctoral program administered in cooperation with the National Academies/National Research Council (NRC).” See NIST, “NIST NRC Postdoctoral Research Associateships Program,” <https://www.nist.gov/iaao/academic-affairs-office/nist-nrc-postdoctoral-research-associateships-program>, accessed December 19, 2020.

## Human Resources

Some locations have space limitations to growth, and yet the workload is increasing. There was not a strong sense of the importance of mentoring, although it was stated that a matched mentoring program was not as fruitful as ad hoc mentoring.

Many nonprofits have succession programs in place, and these have strengthened the overall morale as well as provided the feeling that the research legacies created will continue.

**FINDING:** An overarching goal on achieving diversity and inclusion for performance-based, qualified individuals continues to be important. There appears to be an underlying sentiment that the diversity and inclusion policy (across disciplines, genders, ethnic groups) needs to be developed, when in fact, it has been developed and acted upon.<sup>3</sup>

## Enhancing Learning Opportunities for Existing Staff

The measurement field is a fast-paced technical area with novel methods and instruments coming online on a yearly if not monthly basis. Thus, it is important that existing staff have structured or NIST-endorsed avenues to grow and expand their knowledge base. Considerations include offering sabbatical-like opportunities at other governmental agencies and universities (locally and globally). “Changes in duty station” that permit staff to pursue rotations through other NIST divisions, within BMD, or at nearby universities would also fulfill this need. Short industry-based learning experiences might further enhance the ability of NIST to understand and serve the needs of industry. Given that BMD is within the fourth largest biopharma zone in the United States, it has a geographical advantage in establishing unique educational experiences on which it might capitalize. The new “virtual” environment provides a basis whereby BMD staff could maintain a significant presence at NIST while on a learning opportunity or rotation.

## Enhance Diversity to Enhance Expertise and Problem Solving

There is now ample evidence that diverse teams with varying experience and backgrounds provide better outcomes in problem solving than nondiverse groups.<sup>4,5</sup> Additional viewpoints and backgrounds provide the basis for creative solutions to tough problems. To this end, BMD can strive for increased diversity in its workforce. A clear structure with strategies and milestones would be of value. Discussions with young, mid-career, and senior researchers further illuminated how the staffing, retention, and diversity of the NIST’s outstanding research staff needs to be addressed.

## DISSEMINATION OF OUTPUTS

### Accomplishments

The BMD, as noted earlier, has shown excellence at all levels of dissemination—publications, reports, reference materials, and workshops. BMD researchers have published 174 papers since 2017, many in top-tier peer-reviewed journals. In addressing the NIST mission, they have produced 18

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<sup>3</sup> NIST, 2019, “Inclusivity at NIST: Recent Actions Supporting Equity in Career Advancement at NIST,” presentation to the Visiting Committee on Advanced Technology, October 24, Gaithersburg, MD.

<sup>4</sup> L. Hong and S.E. Page, 2004, “Groups of Diverse Problem Solvers Can Outperform Groups of High-Ability Problem Solvers,” *Proceedings of the National Academy of Sciences U.S.A.* 101(46): 16385–16389.

<sup>5</sup> K.W. Phillips, 2014, “How Diversity Works,” *Scientific American* 311(4): 42-47.

reference materials and three standard reference data libraries. These reference standards include NISTmAb 8671, RM 8634 for particle sizing, and the SARS-CoV-2 research-grade test material RGTM 10169.

Recent high-impact areas that deserve particular recognition include the licensing of BMD's protein sequencing technology to QuantumSi. BMD members also continue to be highly productive as evidenced by their large number of publications in high-quality journals—*Analytical Chemistry*, *Journal of Proteome Research*, *Clinical Chemistry and Laboratory Medicine*, and *DNA Repair*. This includes a recent top 10 downloaded paper in the *Journal of Forensic Science* which was also a top 5 percent cited paper in Wiley Altimetrics. Other impressive numbers include 100 publications citing NIST mAb with over 200 collaborations and 1,000 units/year sold. Notable evidence of BMD's high expertise and respect within the broader community include BMD's MS library citations, which tally over 7,000/year and its electron ionization (EI) library distribution at 6,000/year. BMD's other numerical attributes are equally impressive, reflecting the expertise of the division's scientists. The industry views BMD with high esteem. This is apparent from its collaborations and CRADAs spanning pharma and analytical/scientific measurement companies. These companies include some of the largest and most well-respected enterprises, such as AstraZeneca, Amgen, Thermo-Fisher, and Agilent. The ability of BMD to lead successful roundtables, workshops, and conferences clearly demonstrates that the scientific community recognizes the value of BMD. Of note are BMD-led interlaboratory measurement comparisons of the NIST mAb involving over 100 industrial, academic, and regulatory participants from around the world, including HDX-MS, glycosylation analysis, higher-order structure assessment by NMR, and a Multi-Attribute Method (MAM) Consortium.

### **Opportunities and Challenges**

Current challenges are how to maintain contact during the current COVID-19 pandemic where contacts must be done virtually, and finding ways to safely carry out in-person training and communications in situations where virtual discussions are insufficient.

## 9

# Chemical Sciences Division

## INTRODUCTION

The work of the Material Measurement Laboratory's (MML's) Chemical Sciences Division (CSD) ranges from inorganic and organic chemical metrology to biochemical and exposure science. There are eight groups, including Inorganic Chemical Metrology, Organic Chemical Metrology, Gas Sensing Metrology, Chemical Informatics, Chemical Process and Nuclear Measurements, Biospecimen Science, Optical Measurements, and Biochemical and Exposure Science. There are approximately 170 scientists, engineers, technicians, and support staff in CSD, with approximately 40 percent women. Among group leaders, 50 percent are women.<sup>1</sup> This diversity is impressive for a research institution, and CSD is to be commended.

## ASSESSMENT OF TECHNICAL PROGRAMS

In general, CSD presented work of very high quality both in presentation and scientific content. The speakers were enthusiastic, knowledgeable, and were able to tell the big picture of their story. The presentations included the full breadth of career levels.

### Accomplishments

The Inorganic Chemical Metrology Group is focused on identifying and quantifying inorganic species via a range of analytical methods, including gravimetric analysis, mass spectrometry, optical spectroscopy, X-ray spectroscopy, isotope ratio mass spectrometry, and electrochemical analyses. In addition to pushing the boundaries of established techniques, it is also tasked with developing new techniques and with developing and maintaining primary inorganic reference materials and standards. Recent achievements of note include the Avogadro Project,<sup>2</sup> enabling the kilogram (kg) standard to be redefined, and the development of single-particle inductively coupled plasma mass spectrometry (ICP-MS), including reference materials for calibration.

The Organic Chemical Metrology Group is focused on identifying and quantifying organic species using mass spectrometric, chromatographic, nuclear magnetic resonance, and infrared spectroscopic techniques. It is responsible for (1) preparing and maintaining organic standards and reference materials and (2) improving existing analytical methods and developing new methods. It provides measurement services and develop quality assurance programs for organic analytes. In addition to core areas focusing on food science and forensics, it is also contributing to emerging areas, such as

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<sup>1</sup> Carlos Gonzalez, NIST, 2020, "Chemical Sciences Division," presentation to the panel, September 9.

<sup>2</sup> Savelas Rabb, Inorganic Chemical Metrology Group, NIST, 2020, "The Avogadro Project," presentation to the panel, September 29.

metabolite analysis (metabolomics), cannabinoid quantification, and PFAS (per- and polyfluorinated alkyl substances) standards and analysis.

The Gas Sensing Metrology Group evaluates, develops, and applies measurement technologies for the analysis of gaseous samples and maintains reference data and reference materials that are critically important for measurements of gaseous samples throughout industry, academia, and government. The group also constructs and deploys the NIST Standard Reference Photometer (SRP). The group collaborates with the Optical Measurements Group on the use of some impressive optical spectroscopy methodologies, which can be used for measurement of ultratrace gas levels and even for distinguishing isotopes of gasses.

The Chemical Informatics Group maintains reference databases containing both measured and computed values and carries out computations, simulations, and informatics studies that predict chemical and physical properties and provide a better understanding of complex systems. Recent projects of note include the development of FEASST (Free Energy and Advanced Sampling Simulation Toolkit), a suite of tools for enhancing bottom-up prediction of physical and chemical properties; LipidQC, a validation tool for lipidomics; and a variety of databases, including Visual Mass-Spec Share, Computational Chemistry Comparison, and Benchmark Database and the NIST ARPA-E Database of Novel and Emergent Adsorbent Materials.

The Chemical Process and Nuclear Measurements group brings together expertise and instrumentation to study time-dependent chemical phenomena and possesses a number of capabilities that are both rarely encountered and highly valuable. The group studies high-temperature diffusion coefficients, which are important for developing improved refrigerants. It has a longstanding expertise in studying the transport of lithium ions within batteries using neutron depth profiling, and has strength in the study of high-temperature chemical kinetics, which is important for developing improved gas processes, fire suppressants, and biofuels. The group has expertise in atmospheric chemistry (e.g., estimation of the lifetime of industrial pollutants in the atmosphere) and in measuring heterogeneous systems (e.g., aerosols and thin films). It has significant expertise in proteomics, metabolomics, and lipidomics, in partnership with Measurement Services and the Chemical Informatics Groups, and is working to integrate these into a generalized “OMICS” expertise.

The Biospecimen Science Group focuses on maintaining and operating the biorepository for NIST, primarily of marine life. The biorepository has over 100,000 specimens, which enables long-term tracking of pollutants as well as identification of emerging pollutants, and the group also maintains the cryogenic reference material preparation facility. The biorepository provides national and international importance not only as a place to store and track long-term and new contaminants, but also in establishing proper cradle-to-grave procedures for biospecimens and associated data. Staff are in South Carolina at the Hollings Marine Laboratory and have extensive collaborations with nearby institutions, including the National Oceanic and Atmospheric Administration and the South Carolina Department of Natural Resources

The Optical Measurements Group is a spin-off of the gas metrology group with a focus on developing optical sensing technologies—from the ultraviolet (UV) to the infrared (IR)—for identifying and measuring analytes, as well as collecting and disseminating reference data such as in the High Resolution Transmission Molecular Absorption Database (HITRAN). It performs core functions in quantifying and standardizing greenhouse gas measurements in the environment and is developing techniques to pin isotope ratio scales to SI units, thereby obviating the need for calibration. A notable recent achievement is the development and commercialization of a benchtop  $^{14}\text{C}$  (carbon-14) instrument for applications in forensic analysis, radiocarbon dating, and emissions monitoring.

The Biochemical and Exposure Science Group focuses on the impact of contaminants and pollutants on human and marine health at the endocrine, metabolic, and proteomic level. It operates the Center for Marine Debris Research in Hawaii in collaboration with Hawaii Pacific University, and the Hollings Marine Laboratory NMR spectroscopy and mass spectrometer facilities in South Carolina. Omics and NMR characterization are critical to its mission and it has current focus areas on PFAS and plastics. As part of the exposure program, it maintains 260 SRMs and, in addition to its established

activities, it is also part of the response team of major events, such as the Deepwater Horizon oil spill. The group is also developing best metrological practices for the marine plastics field. Further, the exposure program underpins other federal programs including the Centers for Disease Control and Prevention, the National Institutes of Health, and the Department of Defense. The two groups actively host undergraduates, graduate students, and postdocs through a variety of mechanisms and have seven publications in peer-reviewed journals, with some in high-impact journals.

### **Challenges and Opportunities**

CSD is as noted organized into eight groups, some of them with more than one team. There was a lack of connection between many of the activities in CSD as presented. There is an opportunity for CSD leadership to spend the time crafting a story that would highlight the connections between all teams, or bin the teams into groups in such a way as to provide some level of connection. It may also be worth considering splitting the large groups that have more common alignment or putting some of the teams in other groups where there is alignment. This suggestion may help staff see their place in the organization more clearly. It would also enable CSD leadership to more concisely tell their story.

**RECOMMENDATION 9-1:** The Chemical Sciences Division (CSD) should consider administrative changes to give greater definition to connectivity among the division’s scientists, including binning the teams in CSD to make commonalities with other groups more apparent; and, as warranted, splitting larger divisions and aggregating the groups into new divisions where similarities are strongest.

## **PORTFOLIO OF SCIENTIFIC EXPERTISE**

### **Accomplishments**

There was scientific excellence in every area presented to the panel, and in some cases, this expertise was truly exceptional (e.g., spICP-MS [single-particle inductively coupled plasma mass spectrometry], gas metrology, and the preparation and maintenance of reference standards). There was also clearly growing expertise in the early-career staff. This expertise supported the technical programs very well, with demonstrated deep expertise, as well as broad expertise within the division, as well as within individuals within the division.

Beyond current expertise, there was an eagerness to embrace new technology areas. Bringing computations and data science to bear on experimental problems is a demonstration of this, as is the developing metrology of marine-based plastics.

### **Challenges and Opportunities**

There appears to be an increasing number of activities in CSD without a corresponding increase in resources. This can put an organization at risk of burnout or not meeting deliverables. The MML does not appear to have a clear strategy for dealing with this challenging situation, which seems to lead to some angst among the workforce over funding and resources. There was a recent effort to “weed the garden” and remove some SRMs that were no longer selling or no longer profitable to maintain. The leadership may find it useful to carry out similar culls throughout the organization to identify potential cost savings. It may be helpful for CSD managers to network with their peers in industry, who have become very adept at cost saving measures in recent years, and who could be a good source of relevant best practices.

Retraining was also seen as a challenge for many—to either stay abreast of the field, or to reinvent themselves into a new area. If a sabbatical program in which more senior MML employees rotate to national laboratories, industry, or academia were possible and mutually beneficial, this could serve in retraining as well as increasing MML visibility. This “mixing” will undoubtedly lead to the attrition of some MML workers, but increasing the visibility may also have a two-way effect. Absent this, removing some of the barriers to working with outside people (industry), such as better accessibility to virtual teleconference software options, is essential.

**RECOMMENDATION 9-2:** The Chemical Sciences Division should evaluate its portfolio to determine the fit to Material Measurement Laboratory’s (MML’s) strategy with a view toward adoption of a “steady state” economic model in which new costs are paid for by pruning existing operations. Alternatively, MML could adopt a “pay as you go” model in which they would add new programs, instrumentation, employees, and so forth as new funds become available, or by intentionally pursuing external funding in strategic areas.

## ADEQUACY OF FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

### Accomplishments

CSD is home to unique facilities, including the NIST Biorepository, the Facility for Adsorbent Characterization and Testing (FACT), and Neutron Activation for Elemental Analysis. In addition to specialized facilities and instrumentation, CSD also maintains a wide range of instrumentation for routine analyses. Recently, CSD has started to consider the benefits of shared facilities as a means to curtail costs.

Staff at CSD are top experts in what they do, and they manage legacy collections and work to improve performance of established measurement techniques while also developing new standards, sampling methods, and analytical techniques. Models in which scientists work at CSD while employed by other agencies, such as the Intergovernmental Personnel Act, provide an excellent means for expanding capabilities and research directions without incurring personnel costs. In particular, such mechanisms may provide a means for National Research Council postdocs to continue to perform research at CSD after their fellowship period without becoming a staff member.

**FINDING:** The Chemical Sciences Division has forged strong bonds with a number of federal agencies, industries, and academic institutions that facilitate research through access to specialized instrumentation and expertise. Regarding staff, the Intergovernmental Personnel Act and NRC postdocs program are examples of liaisons that are critical to collaborative research and the mission of CSD.

### Challenges and Opportunities

In recent years, funding available for NIST operations—through the combination of government appropriation (including other agency [OA] funding), income from cooperative research and development agreements (CRADAs), and sale of reference materials—appears to have been flat, yet a variety of factors are contributing to escalating costs for running the division, including the following: ongoing expansion of programs and technology areas; ongoing addition of new instrumentation types; need to replace aging instrumentation; maintaining an expanding fleet of instrumentation; maintaining an aging physical plant and infrastructure for carrying out research; curating sample collections and databases that are not adequately provided for otherwise; and, lastly, escalating labor costs as labor rates rise and as seniority for existing workers increases.



## Facilities and Equipment

The availability of space “to grow” is lacking in CSD, both at the main (Gaithersburg) facility and at the Hollings Marine Laboratory. More problematic is the fact that space is getting tight for existing programs. Notably, both the Gas Metrology and Biological Specimen groups noted that they are running out of space for storing gas and biological specimen samples. As these pertain to core functions of CSD, it is imperative to start formulating a plan now for what to do when capacity is reached.

Aging equipment was a common concern for CSD. There does not seem to be a clear path by which instrumentation is decided upon, acquired, maintained, and shared, but developing this plan is important going forward. It will be important that instrumentation be differentiated between that dedicated to a specific laboratory function (i.e., not-shared, typically due to specialization and/or because critical functionality could be compromised by open access) and general use. Centralization of general use instrumentation in a core facility would have the dual benefit of ensuring that instrumentation use is maximized while enabling maintenance and training to be conducted by a small cadre of core staff, thereby freeing up scientific staff to pursue research. Re-charge mechanisms may be considered as a means to offset routine maintenance and fund support staff. Looking at and adopting best practices in other industries and national laboratories could provide a way to do “more with less.” Scientists have the opportunity to take advantage of collaborations and user facilities to expand the access to instrumentation while reducing the need for a large capital outlay. Acquisition of instrumentation on credit is not a viable long-term strategy and is best employed only as a last resort. Decisions on new research directions must be considered in the context of existing infrastructure, with new directions requiring expensive capital outlays to be weighed against essential or core functions.

The Chemical Informatics Group noted a shortage of computational power available to it. Any infrastructure planning at higher levels of the organization might weigh the cost and merits of significant expansion of computational facilities against other approaches involving accessing existing computational resources through partner organizations. The group also pointed out that being at the cutting edge of this field relies on access to big data, which in the field of measurement science translates to having ready access to the results generated by high-throughput experimentation and high-throughput analysis, neither of which is a current strength within the organization. As building these capabilities will be both slow and costly, the team is urged to investigate opportunities for partnering with existing expertise in these areas to infuse current developments in this rapidly growing field with MML expertise.

The procurement process or what might be called the “business of government” is another factor that significantly reduces the ability of scientists to do work. It would be useful for the business arm to consider the value of lost research time that accrues when instruments and facilities remain un-repaired or critical parts/consumables are not available within a reasonable period of time.

**FINDING:** The appropriated funds out of general taxpayer revenues (the STRS is one such account) is for the purposes of performing research and preparing and maintaining standards. Bureaucratic processes can unnecessarily impede mission progress. Cost-benefit analysis that values time devoted to research can elucidate this. A survey of how staff spend their time could assist management in quantifying this loss.

**RECOMMENDATION 9-3:** The MML should create an instrumentation strategic plan as a useful mechanism to define the current status of instruments via a census (item, age, location, status, responsible person, availability) and prioritization of new instrumentation, as well as identify internal and external support (funds). The MML should also consider developing a plan for maintenance and eventual instrument replacement (where needed) as well as a means of relocating or repurposing underutilized resources.

## **Human Resources**

Critical functions core to the NIST mission are in some cases handled by a very small group of individuals with unique capabilities. This cadre needs to be broadened to ensure retention of institutional memory. This could potentially be achieved by some degree of cross-training and/or rotations, thereby ensuring that key knowledge is not limited to a single set of hands. Broadening the capabilities is expected to lead to new ideas and projects as well as collaborations, making better use of the human capital.

NRC postdoctoral fellows would benefit from more mentoring and professional development opportunities. The fellows seem to be pre-occupied with finding a “path to permanency” at NIST rather than considering the training as a stepping-stone to different opportunities in academia, industry, etc. Formation of an alumni network that includes prior NRC postdocs who took different paths and were successful would provide a means for postdocs to explore the opportunity space, expand their network and find mentors. By the same token, since NRC postdocs are admitted based on an original research project, there is a perception that they are there to do “research” while permanent staff run the laboratories and perform core functions. Such core functions may not have a quantifiable output (such as papers). Publication output is often considered an empirical sign of success for postdocs, so the emphasis on research is understandable. However, opportunities for senior scientists to engage in research, and for NRC postdocs to engage in key laboratory functions, is important for professional development and for diversification of expertise.

## **DISSEMINATION OF OUTPUTS**

### **Accomplishments**

During the period 2017 to 2019, CSD produced approximately 170 external, peer-reviewed publications, 100 NIST reports, 12 data products, and 4 patents. The group produced 70 percent of NIST SRMs (1,000) and 64 reference photometers. In addition, CSD arranged one workshop (Food Safety), and CSD personnel served on 50 national and international standards committees, including 12 leadership positions.

### **Challenges and Opportunities**

Publication output for a group of approximately 170 workers is lower than expected, although a number of employees in the group are working primarily on the preparation of SRMs, which leads to fewer publication opportunities. Nevertheless, the output of peer-reviewed publications seems to be lower than in the previous review period for this group (~2 publications/employee), warranting a closer look at the factors contributing to this decrease.

There is an opportunity for increasing awareness of the importance of the mission of CSD and MML to the science community within the United States as well as to the general public. The ability of CSD staff was impressive at conveying passion and a “big picture” perspective when describing their research, suggesting that CSD consider ways that some of this content can be packaged for presentation that would inform both experts and the general public—everything from scientific lectures to YouTube videos. Notably, the “Cover smart. Do your part. Slow the spread”<sup>3</sup> you-tube video showing how masks limit airflow droplet ejection was a great example of bringing science to the people at a critical time. Note

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<sup>3</sup> See NIST, 2020, “Cover Smart. Do Your Part. Slow the Spread,” video, June 12, <https://youtu.be/sRIdkWKcRbo>.

that while NIST has a YouTube channel, videos range from highly technical for professional scientists and engineers to highly accessible for the general public, with no clear notation for the intended audience.

The Food Safety Workshop<sup>4</sup> in October 2019 was a clear success, but there would have been benefits to convening additional workshops during the 3-year period since the previous review. Going forward, an increasing number of shorter virtual workshops that address key areas of emerging concern linked to the CSD mission may be warranted. While no data were presented relating to CSD employees presenting their work at major scientific conferences, opportunities nonetheless exist for increasing the output of NIST by showcasing a select group of cutting-edge research results along with attending and presenting at major conferences (MRS, ACS, etc.)

Finally, there were opportunities for CSD members to collaborate more closely with other MML divisions and to play a greater role in articulating the MML mission to the outside world. There are also opportunities for CSD to develop stronger ties with the pool of NIST postdoc alumni—both NRC postdocs and NIST associate postdocs. This large cohort of researchers who know NIST well have now moved on into a variety of positions within large industry, government laboratories, small business, and academia. This offers a very valuable network to collect input on emerging areas of concern, problems of note, and feedback on the adoption and implementation of CSD and NIST efforts within the outside world. In addition, by celebrating this cadre of postdoc alumni, CSD would be clearly showing that there are pathways to successful careers for postdocs that lie outside of the NIST organization, which may help to alleviate some of the anxiety that was noted among the postdoc and early-career researchers who portrayed conversion of postdoc to a permanent NIST position as the most important criterion for success.

**RECOMMENDATION 9-4:** The Chemical Sciences Division (CSD) should remain in contact with postdocs (both National Research Council and Associate) and other categories of associates who have left CSD as a way of collecting input on emerging areas of concern, problems of note, and feedback on the adoption and implementation of CSD and Material Measurement Laboratory efforts.

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<sup>4</sup> For further information, see NIST, “NIST Food Safety Workshop,” April 22, 2020, <https://www.nist.gov/news-events/events/2019/10/nist-food-safety-workshop>.

## 10

### Applied Chemicals and Materials

#### INTRODUCTION

The Material Measurement Laboratory's (MML's) Applied Chemicals and Materials Division (ACMD), located in Boulder, Colorado, "characterizes the properties and structures of industrially important fluids and materials." Its work "provides a diverse stakeholder community with innovative measurements and models and critically evaluated data, leading to improved processes and better products, as well as new and improved standards."<sup>1</sup> The ACMD is organized into the following five groups:

- Fatigue and Fracture Group
- Fluid Characterization Group
- Nanoscale Reliability Group
- Thermodynamics Research Center Group
- Thermophysical Properties of Fluids Group

The division chief and four of the five group leaders are new in their positions with the same group structure as in 2017, so it is presumed that the organization is in a state of flux.

Many of the individual projects in these groups are organized for either historical or administrative convenience, in contrast with unifying technical or methodological themes based on the MML mission statement. The division covers a number of long-standing "curator" functions such as the Charpy Verification Program and the REFPROP (Reference Fluid Thermodynamic and Transport Properties) database, which are central to the NIST mission but which dilute the scientific resources needed to maintain leadership in new areas of measurement science.

The ACMD covers all states of matter (gases, liquids, and solids, excepting only plasmas), crosscutting with many industries. As such, the programs are extremely broad. Nearly every project reviewed would fit well into another of the MML divisions, if the Boulder personnel were co-located with the Gaithersburg personnel. Even the title of ACMD covers everything from the applied (curator or legacy) programs through all states of matter be it chemical, biological, or materials. This was also evident in the organization of the presentations, which did not follow the group structure of the division.

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<sup>1</sup> John Perkins, NIST, 2020, "Applied Chemicals and Materials Division: Overview and Introduction," presentation to the panel, September 9.

## ASSESSMENT OF TECHNICAL PROGRAMS

### Accomplishments

One third of the projects are of excellent quality with high-risk/high-impact potential following the recommendations of the 2017 review of the MML.<sup>2</sup> Two notable examples include improved measurement strategies to obtain more accurate thermophysical material properties and cannabis vapor detection.

Other programs are of excellent or good quality but might maintain focus more on the mission statement of the MML. Database (standard reference data or “SRD”) and standard reference material (SRM) activities are mission critical but use resources that limit activities in high risk programs. ACMD must extract full value from clients using these SRMs and databases to free up scientific resources for new projects.

The ACMD has a long history of excellence in thermodynamics of fluids and thermophysical properties. This tradition is maintained in several very strong programs. These seek to use advanced computational and laboratory measurement techniques to make major advances in the accuracy of thermodynamic data. The calculation and measurement of enthalpies of formation are fundamental to nearly all fields of chemistry and materials, as this information contains the strength of the chemical bonds between atoms in these ever more complex molecules. Traditionally the best thermochemical measurements were accurate to no better than 5 percent, but the advanced computational (quantum chemical) and measurement (NMR) methodologies being developed by ACMD are achieving accuracies of 2 percent. This will open new avenues in computational materials science that have yet to be imagined.

Worldwide, there are only a handful of examples of new materials being designed computationally prior to being discovered experimentally in the laboratory. With more accurate thermophysical data, the ability to computationally design new materials prior to synthesizing the material in the laboratory will provide breakthrough methodologies in materials design and remove the empiricism that has ruled the past 100 years. Greater accuracy in thermophysical calculations and measurements will be one of the great scientific accomplishments of the first half of the 21st century. NIST’s AMCD is leading the way in establishing both new computational methods and unique experimental methods that exceed the accuracy of past methods. The computational methods open pathways that are not available experimentally for many new materials.

In the area of vapor science for forensics and public safety, development of a breath-analyzer for Cannabis involves 8 orders of magnitude greater sensitivity than current alcohol breath-analyzers. This requires a multi-prong methodology involving unproven techniques. This project started as a NIST internal program that has expanded to U.S. Department of Justice funding because of the national need. Initial results show promise of meeting the aggressive high-risk goals.

### Challenges and Opportunities

Some ACMD programs are “legacy” in nature (low risk, high monetary value) that utilize headcount and resources to maintain, for example, Charpy standards (SRM) and REFPROP (SRD).

High-risk programs that explore new methodologies to obtain legacy SRM properties would improve the technical program portfolio and add to the high-risk portfolio. There is a conundrum in that a successful high-risk project would eliminate a significant source of funding from the legacy SRMs. But to ignore the opportunity means someone else will take away the legacy program with a new less invasive

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<sup>2</sup> National Academies of Sciences, Engineering, and Medicine (NASEM), 2017, *An Assessment of the National Institute of Standards and Technology Material Measurement Laboratory: Fiscal Year 2017*, Washington, DC: The National Academies Press.

methodology. It would be better for ACMD to lead in improving on this demonstrated national need rather than have another country take the standard away from the United States.

Adding additional experimental methods (e.g., microwave or other electromagnetic measurements for evaluating thermodynamic properties) is an area for which the MML has extensive expertise and can add to the methods being employed in ACMD.

The area of additive manufacturing is high profile, but the MML work, both within ACMD and in other divisions, appears disjointed and is not focused on the MML mission statement.

A number of ACMD projects utilize the outstanding capabilities of NIST in making precision measurements, but the individual projects appear to be driven by client needs rather than fulfilling the MML mission. Attempts must be made to coordinate client needs with the MML mission; otherwise, ACMD risks becoming a high-class service laboratory rather than a leader in measurement technologies.

### **Improved Accuracy of Thermophysical Data**

While NIST and a few other laboratories are making progress in obtaining more accurate thermophysical data, the challenge is to communicate the availability of these new methodologies and the potential uses of such information in advancing new materials design. NIST can do this by hosting or encouraging workshops that highlight the new methodologies with examples where the greater accuracy can make a difference and improve time to market for new materials.

### **Vapor Science for Forensics and Public Safety**

This is a high-risk project but one for which NIST researchers are highly qualified. Challenges include working on regulated substances; ability to administer a multi-year program with only year-to-year funding, especially with 2-year postdocs.

## **PORTFOLIO OF SCIENTIFIC EXPERTISE**

### **Accomplishments**

Since the time of the 2017 report,<sup>3</sup> ACMD has realized a budget growth of 18 percent from \$16.8 million to \$19.9 million with the majority of growth coming from services (\$1.1 million) and agency interactions (\$1.9 million). ACMD has used this funding to support significant scientific expertise.

The ACMD, with 58 scientists (an increase of 7 or 14 percent from the 2017 reporting period), has demonstrated impressive productivity in scientific publications, standards interactions, intellectual property activity, and customer engagement. As noted previously, publication frequency is averaging over 1.3 articles per year per scientist. Of significance is ACMD personnel participation in 44 standards committees with leadership positions in 16 of these committees. It is critical that NIST and ACMD remain in the forefront of these standards committees to better initiate, evaluate, and maintain the strategies for industry standards that impact U.S. manufacturing needs.

Customer engagement is viewed as a key metric for ACMD. ACMD is active in multiple customer interactions where the customer is industry within the United States in the form of either cooperative research and development agreements (CRADAs) or non-disclosure agreements (NDAs). In particular, the NDA approach is a proven path to commercialization of NIST intellectual activities.

Scientific expertise is also viewed from the perspective of initiating new and likely high-risk projects. Two ACMD programs that demonstrated this perspective were vapor forensics for cannabis

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<sup>3</sup> Ibid.

detection and advanced NMR strategies or microwave strategies for the determination of thermodynamic properties of materials.

### **Opportunities and Challenges**

Interaction and/or collaboration between the two main NIST sites (Gaithersburg and Boulder) was not emphasized in the ACMD presentations. Formalizing such interactions would be beneficial to the ACMD goals.

One source of acquiring talent for ACMD is a continued and more aggressive effort in sponsoring positions for the National Research Council (NRC) Research Associateship Program (RAP). This is one of the most efficient ways of initiating new and high-risk programs.

As noted, the growth of associate positions in the ACMD was unusually high during this last 3-year period (from 16 to 29 persons, or an 81 percent increase). Three of the associates are paid to work for NIST full time. Most of the remaining 26 are external collaborators. Since many of these positions are subject to renewal on a 2-year cycle, ACMD must establish a plan to retain or renew talent to sustain existing programs and/or create new programs.

## **ADEQUACY OF FACILITIES, EQUIPMENT, AND HUMAN RESOURCES**

### **Accomplishments**

There have been no major new facilities in the Boulder Campus or at least none were described during the review. The major concern repeated numerous times was the housing in 50-year old laboratories. This may be a concern, but it is beyond the charge of the panel review.

The Nanoscale Reliability Group within ACMD noted the “aging” of key characterization equipment, including the following: focused ion beam (FIB) sample preparation tool; transmission electron microscope (TEM); and field emission scanning electron microscope/electron backscatter diffraction microscope. A capital equipment replacement plan for these critical tools was not presented.

Over the last 3-year review period, ACMD showed total staff growth of 23 percent (76 to 94) with number of scientists increasing 14 percent (51 to 58) and number of associates increasing 81 percent (16 to 29). The growth rate for associates appears unusually high when compared to the MML total number of associates actually decreasing by 6 percent (919 to 858).

### **Opportunities and Challenges**

The ACMD dependence on a significant increase in associate staff for new programs may lead to potential program continuity issues as the tenure for short-term employees ends. It was apparent that tenure prospects have not been adequately conveyed to associates. ACMD may not succeed in sustaining additional program growth through reliance on increases in future associates. As associates complete their terms, new programs will need to be initiated and old programs ended.

If capital equipment replacement for aging tools is mission critical, then this might best be accompanied by a priority list provided to higher organizational management. ACMD noted potential equipment sources from the U.S. government surplus listings.

**RECOMMENDATION 10-1:** The Applied Chemicals and Materials Division should create a capital equipment replacement plan that considers also the requirements for space and ongoing maintenance.

## DISSEMINATION OF OUTPUTS

### Accomplishments

The ACMD has done a good job of disseminating its output in several different ways. The ACMD personnel publish substantially in the open literature, with 222 papers in archival journals, 26 in conference proceedings, 18 book chapters, and 20 reports from April 2017 to August 2020. This amounts to a journal publication rate of 1.3 papers per researcher per year; this is about average in comparison with other research facilities, including universities and national laboratories. The ACMD staff members actively participate in seminars, workshops, and conference presentations with over 102 invited presentations in the last 3 years. The ACMD has worked closely with a variety of agencies, such as the American Society for Testing and Materials (ASTM), the International Organization for Standardization (ISO), and the American National Standards Institute (ANSI), in developing standards. As noted, the staff participates in as many as 44 standards committees with several staff members assuming leadership positions on these committees.

The ACMD does an excellent job of disseminating its output in the traditional area. Dissemination of output by the Thermodynamics Research Center is excellent. The Fatigue and Fracture Group disseminates its work through its influence on codes and standards for testing and designing with structural materials. There are several favorable examples of programs driven by stakeholder needs, most notably the Charpy Impact Machine Verification Program and the Thermophysical Properties of Fluids. The Charpy Impact Machine Verification Program serves over 1,200 manufacturers and users worldwide, whose Charpy Testing Machines are being certified by the ACMD for compliance with ASTM and ISO standards, and is an excellent example of monitoring stakeholder use of outputs through SRMs. It has remained the leading NIST SRM year after year with worldwide impact. The ACMD's thermodynamic and chemical property data sets assist stakeholders and, in some cases, are an enabler of commercial process-modeling software. The ACMD validates the impact of its work through database (SRDs) access and SRMs sales; there were 17 SRM/RM activities and 14 SRD activities in the division. One example for the impact validation of the SRD programs is the REFPROP (Reference Fluid Thermodynamic and Transport Properties) equation of state engine with 1,423 annual licenses.

The ACMD has been awarded 10 patents with 18 additional invention disclosures and patent applications over the past 3 years.

Overall, the ACMD does an excellent job of disseminating its output to all stakeholders.

### Opportunities and Challenges

ACMD has created significant impact with key SRDs and SRMs. The challenge for ACMD is to properly value their SRD/SRM portfolio so that new programs can be initiated, in particular programs that explore new solutions to legacy SRM strategies.

While the ACMD is making progress in obtaining more accurate thermophysical data, the challenge is to communicate the availability of these new methodologies and the potential uses of such information in advancing new materials design. MML and the ACMD in particular can do this by hosting or encouraging workshops that highlight the new methodologies with examples where the greater accuracy can make a difference and improve time to market for new materials.

Overall, the ACMD does an excellent job of disseminating the outputs of its technical work. One way ACMD could improve its dissemination would be through establishing an exchange program between ACMD personnel and organizations in industry, universities, and national laboratories—both to and from ACMD. Universities and other organizations have benefited from these kinds of exchange programs in facilitating and expanding dissemination and the enhancement of staff.



## CONCLUSIONS AND RECOMMENDATIONS

ACMD has SRD and SRM activities that utilize personnel resources to maintain legacy standards. Initiating new programs to examine replacement or improvement strategies for these standards activities would position ACMD at the forefront of the next generation of standards requirements. Properly valuing the SRD and SRM activities would create revenue to support such activities.

**RECOMMENDATION 10-2:** The Applied Chemicals and Materials Division should take steps to realize the true value of standard reference data and standard reference materials thereby enabling revenue for growth of new programs.

Over the past 15-20 years, NIST's MML has evolved from a Materials Science and Engineering focused research laboratory to become the nation's premier material measurement laboratory specializing in precision measurement methodologies and standards, supporting industry in the chemical, biological, and materials fields. ACMD has the same breadth of industries as does the larger MML, with an outstanding history of precision chemical, thermodynamic, and mechanical property measurements. Virtually all of the projects within ACMD fit within the competencies of divisions housed in Gaithersburg, yet it is not clear that the interaction between these two physically distant laboratories are as close as they might be in an era where virtual discussion is becoming the norm.

**RECOMMENDATION 10-3:** MML should (1) clearly define the Applied Chemicals and Materials Division's (ACMD's) mission and how ACMD aligns within the Material Measurement Laboratory mission; and (2) integrate teams more closely with corresponding efforts in NIST Gaithersburg facilities.

High-risk project activity is one measure of the technical vitality of an organization. High-risk projects include—for example, vapor forensics for public safety and NMR and microwave techniques for thermodynamic property characterization.

**RECOMMENDATION 10-4:** The Applied Chemicals and Materials Division should continue to increase the number of high-risk projects.

## 11

### Adoption of 2017 Report

This chapter assesses the extent to which the Material Measurement Laboratory (MML) followed the recommendations made in the previous review by the National Academies<sup>1</sup>—hereafter “the 2017 review.” The sections below include observations on specific recommendations from 2017 that were addressed to the offices and divisions.

#### OFFICE OF REFERENCE MATERIALS

The leadership and staff of the Office of Reference Materials (ORM) have made earnest efforts and significant progress in meeting recommendations in response to the 2017 review. In particular, ORM has greatly improved the e-business tools that are necessary to operate efficiently and effectively to meet customer and market needs. Further, ORM is looking forward to anticipated standard reference material (SRM) needs that arise from new and emerging industry sectors, and is working closely with other NIST units to develop those SRMs. Storage and packaging issues are still significant challenges and ORM recognizes how these needs limit their ability to be responsive to the needs of industry. ORM has made progress working with NIST units to create new SRMs, yet the importance of SRMs to NIST mission is not widely understood by all MML technical staff.

#### OFFICE OF DATA AND INFORMATICS

The Office of Data and Informatics (ODI) has made serious progress in achieving the goals in response to the 2017 report. In the response to the 2017 review, ODI had proposed to push for laboratory-driven science involving instrumentation and detectors and analytics. ODI has introduced efforts to embed data driven metrology into the research workflow at NIST. Laboratory information management system (LIMS) capabilities at NIST have advanced significantly through establishment of a network. The cultural acceptance of doing data driven research is still a challenge. Scientific researchers not familiar with data analytical techniques still question why it is necessary track and keep data. The challenges acknowledged in the 2017 review seem to persist. Initial efforts toward data management plans (DMPs) were uneven, and staff generally consider DMPs to be an administrative burden with no real benefit.

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<sup>1</sup> National Academies of Sciences, Engineering, and Medicine, 2017, *An Assessment of the National Institute of Standards and Technology Material Measurement Laboratory: Fiscal Year 2017*, Washington, DC: The National Academies Press.

## **MATERIALS SCIENCE AND ENGINEERING DIVISION**

In the 2017 review, it was noted in Recommendation 17 that the MML should consider updating the Materials Science and Engineering Division's (MSED's) laboratory equipment for making, processing, and preparing metallic alloys for testing (p. 8). From a higher-level review of future program directions, it appears that MSED is matching strategic direction with functional laboratory capability. MSED should however continue to ensure the alloy melting furnaces been reviewed for atmospheric control and melting capacity both on a heat size and annual capacity basis; give consideration to upgrading the instrumentation of the laboratory rolling mill; and review or upgrade, as appropriate, metallographic preparation facilities in light of existing and new alloys being developed, and the expected amount of metallographic preparation required in the future.

## **MATERIALS MEASUREMENT SCIENCE DIVISION**

The responses to the three findings and recommendations included in the Materials Measurement Science Division (MMSD) section of the 2017 review are appropriate. The MMSD competency database was terminated in 2016. Now inter- and intra-division collaborations are fostered through mechanisms focused around increased awareness and communications regarding division activities. The second recommendation was to consider leveraging the NIST postdoctoral network with a professional development program in order to improve connectivity across NIST and improve transparency of how to succeed, especially for early career staff. A new comprehensive program was launched in fiscal year 2020 to ensure all staff have a clear understanding of how to have a successful experience within MMSD and NIST. The recommendation to consider making the application of the MMSD's experimental design and statistical analysis more uniform has been addressed through working closely with the NIST Statistical Engineering Division.

## **BIOSYSTEMS AND BIOMATERIALS DIVISION**

In the Biosystems and Biomaterials Division (BBD), the review panel noted strong collaborator outreach through consortia, workshops, and leadership participation in international panels and working groups as well as internal collaboration with ODI. Collectively, these activities succeeded in addressing and in some instances likely exceeding the expectations of the recommendations from the 2017 review.

One area that is particularly challenging is the need to monitor for any loss of scientific knowledge. With an escalating workload and a declining number of people, it has become difficult to spend time cross training staff into different areas. For instance, virology and microbiology are becoming very significant and call for expertise in microbes and attendant expertise in fluid mechanics and colloidal science. In such instances, cross training builds depth of knowledge and prepares for such eventualities as can occur when someone leaves (due to another job, governmental policy changes) and another person must fill the role. A similar recommendation (9) was made in the 2017 review (p. 6).

The division conducted the renovations called for in Recommendation 10 of the 2017 review. These however were accompanied by a 20 percent reduction in space.

The issue of cost burden due to agency (NIST) overhead remains, which was Recommendation 11 of the 2017 review (p. 7), and which hinders interagency grants. This could be addressed by a review of this overhead.

## **BIOMOLECULAR MEASUREMENT DIVISION**

The Biomolecular Measurement Division (BMD) has done overall a good job in responding to the recommendations of the 2017 review. The challenge lies in finding resources for maintaining existing infrastructure (leaky roofs, HVAC [heating, ventilation and cooling] in need of repair, etc.) while still being able to update instrumentation capabilities. Buildings on the main campus may have exceeded their “design life” and were otherwise in need of repair. Finding resources to address this is difficult but critical to maintaining infrastructure that is consistent with, and will support operations of exquisitely sensitive instruments, and the brand for excellence that is associated with NIST worldwide.

## **CHEMICAL SCIENCES DIVISION**

The Chemical Sciences Division (CSD) has made important inroads to address the recommendation from the 2017 review. For instance, the administrative staff has undergone a reorganization and several non-PhD staff have been hired to assist with technical support. CSD has also been successful in increasing the numbers of National Research Council (NRC) postdoctoral fellows, thereby enabling new research endeavors.

CSD could continue to work on increasing their visibility and impact through seminar series, serving on panels and “staff exchanges with industry, national laboratories, etc. It can facilitate the retention of current staff by proactively recruiting the best postdoctoral candidates from all groups and establishing a formal process for nominating (and winning) external awards. The ability to update and replace equipment, as well as acquire new capabilities, is another area that CSD could continue to improve.

## **APPLIED CHEMICALS AND MATERIALS DIVISION**

The 2017 review for the Applied Chemicals and Materials Division (ACMD) suggested two recommendations: (1) expanding efforts in high-risk projects and (2) engaging personnel in exchange programs with other organizations in industry, universities, and national laboratories. Significant progress was demonstrated in the first recommendation for high-risk projects as evidenced by several presentations; specifically, in vapor science for forensics and in unique experimental methods for measuring more accurate thermophysical material properties. It is suggested that ACMD continue its effort to move to more high-risk, high-payoff projects. The second recommendation related to exchange programs, while desirable, was not addressed in presentations. Logistics of such exchange programs are not compatible with present national health issues.

## 12

**Conclusions and Recommendations****GENERAL CONCLUSIONS AND RECOMMENDATIONS**

The study identified a number of themes across the Material Measurement Laboratory (MML) divisions and offices regarding the high technical quality of the research, excellence of the scientific staff, strong customer outreach and scientific collaboration, and strong publication and dissemination activities. The recommendations in the following sections are grouped by division or office to provide actionable suggestions that address the unique needs of each; the two or three recommendations judged to be of greatest urgency for each division are included here. There are, in addition, several crosscutting themes that fall within the four items of the panel's statement of task that will be discussed first.

As regards technical adequacy, MML conducts research that is exceptional. It has formal arrangements with renowned institutions such as Brookhaven National Laboratory and, in the IBBR, two campuses of the University of Maryland system. MML notes that areas of new opportunities include bioeconomy and engineering biology, data and artificial intelligence, and the circular economy. The MML has primary responsibility within NIST for standard reference materials (SRMs) and standard reference data (SRD). It maintains critical SRM and SRD and has developed these products in newer areas based on biology. The panel's review showed that as the portfolio of SRM expands into new areas, such as biology, the MML will need to consider how to optimally allocate resources between maintaining legacy SRM versus re-purposing those resources towards SRM and SRD in new and emerging areas.

As regards the portfolio of scientific expertise, the resilience of MML's program to retirements or unforeseen departures could be improved. In some places there needed to be more systematic succession planning to prevent gaps from occurring. Cross-training to provide backup coverage in case the primary cognizant scientist leaves is a further way to protect against disruption. In other instances, retraining to take on emerging issues requiring different disciplinary knowledge was lacking.

With respect to the adequacy of facilities and equipment, the research equipment utilized in the divisions of the MML supports or enables the delivery of the MML mission. The purchase, renewal and maintenance of such equipment—including maintaining the buildings that house them—are effected through a set of business practices and attitudes. The purchasing power of the divisions is impacted first by a 50 percent tax on equipment. This disadvantages equipment purchases for purposes of budget formulation by making the trade-off versus funding an additional staff position or other expenditures more acute. Further, the NIST working capital fund model for purchase of new equipment requires payback for any purchase from annual operating funds. The MML also noted these continuing challenges of aging and outdated building infrastructure and "large" equipment needs and uses.

Complicating this is the ongoing challenge in finding resources for maintaining existing infrastructure (leaky roofs, HVAC [heating, ventilation and cooling] in need of repair, etc.). Although, equipment and staff are appropriately prioritized over buildings, there have been instances where failures of the infrastructure compromised equipment and have impact on mission delivery. The buildings on the main NIST campus may have exceeded their design life and are otherwise in need of repair. Finding resources to address this is difficult but critical to maintaining infrastructure that is consistent with, and will support operations of exquisitely sensitive instruments, and the brand for excellence that is associated

with NIST worldwide. This includes modular laboratories that are flexible in use and can be relocated and/or reconfigured within a new room or building.

Lastly, as regards the dissemination of outputs, the MML could benefit from using its network of former postdocs as brand ambassadors, as was indicated in the 2017 review.<sup>1</sup> The research staff continues to make its mark in journals. The laboratory continues to hold an impressive number of convening activities. Its staff are very well represented on federal interagency groups such as the National Science and Technology Council and in NGOs such as the International Organization for Standards (ISO). The MML could benefit from its permanent staff presenting more talks in various forums as a way of maintaining presence.

## DIVISION- AND OFFICE-LEVEL RECOMMENDATIONS

### Office of Reference Materials

**RECOMMENDATION 3-1:** The Office of Reference Materials (ORM) should plan and host a series of topic-focused workshops with participation from industry, academia, and other government organizations to benchmark and identify state-of-the-art business practices, e-commerce tools/platforms, marketing and sales operations, packaging, and other areas critical to its operations. As part of such an undertaking, ORM should assess the appropriateness and feasibility of outsourcing portions of its operations or the expanded use of public-private partnerships to increase efficiency of its operations including standard reference material fabrication, storage (inventory control), packaging, and other critical operations.

**RECOMMENDATION 3-2:** The Office of Reference Materials should develop processes and procedures to strategically select and prioritize the use of working capital funds toward high-demand products, which can maximize the throughput and return value; and examine methods to accelerate and evaluate the development of these new standard reference material products. The evaluation can be used to further promote and/or incentivize the MML division-level SRM development.

**RECOMMENDATION 3-3:** The Office of Reference Materials (ORM) should conduct informational symposia and workshops to better communicate the vital role that ORM plays in the mission of NIST and to highlight success stories. The office should also provide more systematic evaluation feedback and greater incentives for MML division staff to more effectively and efficiently develop new standard reference materials that are aligned with the needs of industry..

### Office of Data and Informatics

**RECOMMENDATION 4-1:** The Material Measurement Laboratory management should promote the concept of “data as an asset” and its associated culture within the Laboratory. With that understanding, management can be expected to advocate and support its adoption throughout the organization, resulting in increased professionalism within NIST, higher quality of output by NIST, increased impact of NIST products on the STEM world, and public perception of NIST as a leader.

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<sup>1</sup> National Academies of Sciences, Engineering, and Medicine, 2017, *An Assessment of the National Institute of Standards and Technology Material Measurement Laboratory: Fiscal Year 2017*, Washington, DC: The National Academies Press.

**RECOMMENDATION 4-2:** The Office of Data and Informatics (ODI) should build out structures for enhancing divisional interactions. One concrete mechanism for this is to create tightly integrated multidisciplinary teams, which include ODI domain expertise as an integral part of a research team. The concept of “research software engineering” has been advocated as one such mechanism for creating research teams that can respond to the centrality of data and computation in a research activity.

**RECOMMENDATION 4-3:** The “software carpentry” program should be expanded to include rotations of postdocs through ODI for more extensive, hands-on guidance. In addition, identifying postdocs in the MML divisions with an understanding of the importance of sound computational techniques and establishing joint mentorship programs with those divisions and ODI would be beneficial.

**RECOMMENDATION 4-4:** The Material Measurement Laboratory should enhance engagement with creation/integration of reference materials.

### **Materials Science and Engineering**

**RECOMMENDATION 5-1:** The Materials Science and Engineering Division (MSED) should consider investment in additional high-performance computing resources to continue the comparative advantage the Thermodynamics and Kinetics group holds. In making such investments, MSED should maintain balance with empirical approaches.

**RECOMMENDATION 5-2:** The Materials Science and Engineering Division should develop a clear articulation of a broad-based strategic plan of the division and state how that plan reflects the overarching strategic plan of the Material Measurement Laboratory.

**RECOMMENDATION 5-3:** The Material Measurement Laboratory (MML) should evaluate how it budgets new equipment purchases and how this figures in to the resource management in its divisions. The MML should further remain aware of the damage to equipment due to flooding and other problems with buildings and facilities.

**RECOMMENDATION 5-4:** The Material Measurement Laboratory should increase its activities aimed at communicating its accomplishments to its customers, collaborators, and audiences. This should include greater effort at highlighting results from the primary work of the laboratory. This could be accomplished using forms of media such as YouTube and improving the effectiveness of the NIST website by adding specific examples of unique and transformative contributions.

### **Materials Measurement Science Division**

**RECOMMENDATION 6-1:** The Materials Measurement Science Division (MMSD) should increase the degree to which it utilizes its customers for feedback on new products and information with regard to emerging opportunities. To this end, the Material Measurement Laboratory should utilize a process for obtaining feedback. MMSD should increase its interaction with the offices managing sales of such products at NIST.

**RECOMMENDATION 6-2:** The Materials Measurement Science Division should evaluate whether to move some of the work of the Materials for Energy and Sustainable Development group (e.g., X-ray Metrology) to another group (e.g., Materials Structure and Data Group) and refocus the former group's efforts on materials data and artificial intelligence approaches.

**RECOMMENDATION 6-3:** The Materials Measurement Science Division should conduct additional intra-divisional collaboration, which might be exploited to add fundamental understanding for the benefit of the research component of the work going forward.

**RECOMMENDATION 6-4:** The management of the Materials Measurement Science Division will need to continue to evaluate and understand the impact of the change in staff numbers and redistribution of workloads. Specifically, there needs to be a shared understanding of the division mission that justifies staff numbers.

**RECOMMENDATION 6-5:** The Materials Measurement Science Division (MMSD) should examine ways to recruit and retain greater numbers of female scientific staff. MMSD staff should all work to enhance the visibility of NIST as a career option through technical meeting/society activities and university interactions. All team members should ensure inclusiveness and assist with career development of the diverse workforce, including the careers of associates and post docs.

**RECOMMENDATION 6-6:** The Materials Measurement Science Division should prioritize the division's needs for upgrading/replacement of equipment and explore centralizing commonly used instrumentation at the division or laboratory level.

### **Biosystems and Biomaterials Division**

**RECOMMENDATION 7-1:** The Biosystems and Biomaterials Division (BBD) should (1) with creativity, develop a business strategy that focuses on BBD's unique products that may include licensing and further consortia for use of BBD products, services, and expertise; (2) strategically place BBD postdoctoral fellows into industry, academia, and other government positions to improve connectivity with outside current and future collaborators and stakeholders; (3) hire or contract with a communications person with YouTube and other media expertise to reach individuals who are searching for BBD-type expertise, products, and research services; and (4) determine how to connect with quality and manufacturing personnel at small and medium-sized companies in targeted industries. Emphasizing NIST BBD leadership, with thoughtfulness and quantification, in BBD program areas should be addressed by BBD leadership and staff to further enhance leadership with collaborators and stakeholders.

**RECOMMENDATION 7-2:** The Biosystems and Biomaterials Division should improve awareness of its products and capabilities, especially within small to medium-size enterprises and companies that are not currently stakeholders because they are in different industries (e.g., agriculture).

**RECOMMENDATION 7-3:** The Material Measurement Laboratory should evaluate whether the square footage assigned the Biosystems and Biomaterials Division is commensurate with the division's current size and mission.



**RECOMMENDATION 7-4:** The Biosystems and Biomaterials Division should provide additional resources in thermodynamics, fluid mechanics, colloidal science, virology, immunology, microbiology, and bioinformatics in a manner commensurate with the increasing importance of these specialties.

**RECOMMENDATION 7-5:** The Biosystems and Biomaterials Division should analyze underserved minority representation among its staff and develop an action plan to address findings both from such study and from NIST's equity disparity studies.

**RECOMMENDATION 7-6:** The Biosystems and Biomaterials Division should develop a plan for outplacing long-tenured postdoctoral fellows into synergistic positions in industry, academia, or government. This plan should include an assessment of what shortfall, if any, this might create in its staffing plans.

**RECOMMENDATION 7-7:** The Biosystems and Biomaterials Division leadership should implement cross-training of staff with intent during each year to mitigate the effects of loss of key staff and ensure continuity.

### **Biomolecular Measurement Division**

**RECOMMENDATION 8-1:** The Biological Measurement Division (BMD) should evaluate its portfolio of expertise of staff with expertise in artificial intelligence and machine learning as applied to the measurement tools specifically in BMD. BMD might want to consider a joint hire with another division to leverage additional expertise and resources, or develop a more centralized collaboration model (i.e., community of practice) to make enhanced use of AI/ML expertise.

**RECOMMENDATION 8-2:** The Biological Measurement Division (BMD) should develop a strategy to assess agriculture, veterinary science, biocatalysis, and environmental and marine research areas as possible opportunities for growth and sources of additional collaborations and funding.

### **Chemical Sciences Division**

**RECOMMENDATION 9-1:** The Chemical Sciences Division (CSD) should consider administrative changes to give greater definition to connectivity among the division's scientists, including binning the teams in CSD to make commonalities with other groups more apparent; and, as warranted, splitting larger divisions and aggregating the groups into new divisions where similarities are strongest.

**RECOMMENDATION 9-2:** The Chemical Sciences Division should evaluate its portfolio to determine the fit to Material Measurement Laboratory's (MML's) strategy with a view toward adoption of a "steady state" economic model in which new costs are paid for by pruning existing operations. Alternatively, MML could adopt a "pay as you go" model in which they would add new programs, instrumentation, employees, and so forth as new funds become available, or by intentionally pursuing external funding in strategic areas.

**RECOMMENDATION 9-3:** The MML should create an instrumentation strategic plan as a useful mechanism to define the current status of instruments via a census (item, age, location, status, responsible person, availability) and prioritization of new instrumentation, as well as identify internal and external support (funds). The MML should also consider developing a plan for maintenance and eventual instrument replacement (where needed) as well as a means of relocating or repurposing underutilized resources.

**RECOMMENDATION 9-4:** The Chemical Sciences Division (CSD) should remain in contact with postdoctoral (NRC and Associate) and other categories of associates who have left CSD as a way of collecting input on emerging areas of concern, problems of note, and feedback on the adoption and implementation of CSD and Material Measurement Laboratory efforts.

### **Applied Chemicals and Materials Division**

**RECOMMENDATION 10-1:** The Applied Chemicals and Materials Division should create a capital equipment replacement plan that considers also the requirements for space and ongoing maintenance.

**RECOMMENDATION 10-2:** The Applied Chemicals and Materials Division should take steps to realize the true value of standard reference data and standard reference materials thereby enabling revenue for growth of new programs.

**RECOMMENDATION 10-3:** MML should (1) clearly define the Applied Chemicals and Materials Division's (ACMD's) mission and how ACMD aligns within the Material Measurement Laboratory mission; and (2) integrate teams more closely with corresponding efforts in NIST Gaithersburg facilities.

**RECOMMENDATION 10-4:** The Applied Chemicals and Materials Division should continue to increase the number of high-risk projects.



## Acronyms

4D STEM	4D scanning transmission electron microscopy
AAFS	American Academy of Forensic Sciences
ACMD	Applied Chemicals and Materials Division
ACS	American Chemical Society
AFM	atomic force microscopy
AMAP	Arctic Monitoring and Assessment Programme
AM Bench	Additive Manufacturing Benchmark Test Series
API	application programming interface
APS	American Physical Society
ARMI	Advanced Regenerative Manufacturing Institute
ARPA-E	Advanced Research Projects Agency-Energy
ASM	American Society of Materials
ASTM	American Society for Testing and Materials
ASTMi	American Society for Testing Materials International
ATB-MII	Advanced Tissue Biofabrication Manufacturing Innovation Institute
ATCC	American Type Culture Collection
BADSS	Business Application Development, Support, and Security Group
BBD	Biosystems and Biomaterials Division
BCARS	broadband coherent anti-Stokes Raman scattering
BMD	Biomolecular Measurement Division
BSL-2	Biosafety Level 2
CALPHAD	Computer Coupling of Phase Diagrams and Thermochemistry
CDC	Centers for Disease Control
CSD	Chemical Sciences Division
cGMP	current Good Manufacturing Practices
CHiMaD	Center for Hierarchical Materials Design
CHO	Chinese Hamster Ovary cells
CLL	chronic lymphocytic leukemia
CODATA	Committee on Data of the International Science Council
CNST	Center for Nanoscale Science and Technology
CRADA	Cooperative Research and Development Agreement

CRP	C-reactive protein
CSD	Chemical Sciences Division
CSTL	Chemical Science and Technology Laboratory
ctDNA	circulating tumor DNA
DARPA	Defense Advanced Research Projects Agency
DFT	density functional theory
DHS	Department of Homeland Security
DMP	data management plan
DNA	deoxyribonucleic acid
DOC	Department of Commerce
DoD	Department of Defense
DOE	Department of Energy
DOJ	Department of Justice
DOT	Department of Transportation
EDRN	Early Detection Research Network
EELS	electron energy-loss spectroscopy
EGFR	epidermal growth factor receptor
ENP	engineered nanoparticle
EPA	Environmental Protection Agency
EPR	Electron Paramagnetic Resonance
ERCC	External RNA Controls Consortium
ERF	equivalent number of reference fluorophores
EXAFS	extended X-ray absorption fine structure
FBI	Federal Bureau of Investigation
FDA	Food and Drug Administration
FIB SEM	focused ion beam scanning electron microscope
FISH	fluorescence in situ hybridization
FIZ	Fachinformationszentrum Karlsruhe
FTE	full-time equivalent
GHS	Globally Harmonized System
GIAB	Genome in a Bottle
GM	General Motors
HER2	human epidermal growth factor receptor 2
HML	Hollings Marine Laboratory
HMP	Human Microbiome Project
IBBR	Institute for Bioscience and Biotechnology Research
ICSD	Inorganic Crystal Structure Database
IFCC	International Federation of Clinical Chemistry and Laboratory Medicine

IgG	immunoglobulin G
IMMSA	International Metagenomics and Microbiome Standards Alliance
InChI	International Chemical Identifier
ISCT	International Society for Cellular Therapy
ISO	International Organization for Standardization
IT	information technology
ITL	Information Technology Laboratory
IUPAC	International Union of Pure and Applied Chemistry
JANAF	Joint Army Navy Airforce
JILA	Joint Institute for Laboratory Astrophysics
JIMB	Joint Initiative for Metrology in Biology
LC-MS	liquid chromatography-mass spectrometry
LIMS	Laboratory Information Management System
Li-ions	lithium-ions
low-GWP	low-global warming potential
mAb	monoclonal antibody
MATES	Multi-Agency Tissue Engineering Science
MCL	Molecular Characterization Laboratory
MDCS	Materials Data Curation System
MEP	Manufacturing Extension Partnership
MGI	Materials Genome Initiative
MIDAS	Management of Institutional Data Assets
miRNA	microRNA
MIT	Massachusetts Institute of Technology
MML	Material Measurement Laboratory
MMSD	Materials Measurement Science Division
MOU	Memorandum of Understanding
MSED	Materials Science and Engineering Division
MSEL	Materials Science and Engineering Laboratory
MTA	Materials Transfer Agreement
NCI	National Cancer Institute
NCI-MATCH	National Cancer Institute, Molecular Analysis for Therapy Choice
NCMC	National Cell Manufacturing Consortium
NDA	nondisclosure agreement
NDP	neutron depth profiling
NERSC	National Energy Research Scientific Computing Center
NGS	next-generation sequencing
NIAID	National Institute of Allergy and Infectious Diseases

NIDCR	National Institute of Dental and Craniofacial Research
NIH	National Institutes of Health
NIIMBL	National Institute for Innovation in Manufacturing Biopharmaceuticals
NIST	National Institute of Standards and Technology
NMR	nuclear magnetic resonance
NNSA	National Nuclear Security Administration
NOAA	National Oceanic and Atmospheric Administration
NRC	National Research Council
NREL	National Renewable Energy Laboratory
NLSL-II	National Synchrotron Light Source II
N-STEP	NIST Science and Technology Entrepreneurship Program
OAR	Open Access to Research
ODI	Office of Data and Informatics
OISM	Office of Information Systems Management
ORM	Office of Reference Materials
OSTP	Office of Science and Technology Policy
PECASE	Presidential Early Career Award for Scientists and Engineers
PLOT-cryo	porous layer open tubular cryoadsorption
PML	Physical Measurement Laboratory
R&D	research and development
REFPROP	Reference Fluid Thermodynamic and Transport Properties Database
RM	reference method
RMP	reference measurement procedure
SAXS	small-angle X-ray scattering
SBSC	Synthetic Biology Standards Consortium
SCB	Standards Coordinating Body
SD	service development
SEM	scanning electron microscopy
SERI	strategic and emerging research initiatives
SMSD	Surface and Microanalysis Science Division
SPRi	surface plasmon resonance imaging
SRD	standard reference data
SRI	standard reference instrument
SRM	standard reference material
STEM	science, technology, engineering, and mathematics
STR	short tandem repeat
TE	tissue engineering
TEM	transmission electron microscopy

TERMIS-AM	Tissue Engineering and Regenerative Medicine International Society-Americas
TMS	The Minerals, Metals, and Materials Society
UMD	University of Maryland
URL	uniform resource locator
U.S. TAG	U.S. Technical Advisory Group
UV-Vis	ultraviolet–visible spectroscopy
WCF	working capital fund
XEDS	Energy-dispersive X-ray Spectroscopy
XRD	X-ray diffraction



