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

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

Committee on NIST Technical Programs

Laboratory Assessments Board

Division on Engineering and Physical Sciences

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PANEL ON REVIEW OF THE MATERIAL MEASUREMENT LABORATORY AT THE NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

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Acknowledgment of Reviewers

This report has been reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise, in accordance with procedures approved by the National Research Council's Report Review Committee. The purpose of this independent review is to provide candid and critical comments that will assist the institution in making its published report as sound as possible and to ensure that the report meets institutional standards for 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 wish to thank the following individuals for their review of this report:

Dennis E. Discher, University of Pennsylvania,
Ian D. Jardine, Fisher Scientific,
Mark H. Kryder, Carnegie Mellon University,
Julia M. Phillips, Sandia National Laboratories,
Alton D. Romig, Jr., Lockheed Martin Aeronautics Company, and
William Tumas, National Renewable Energy Laboratory.

Although the reviewers listed above have provided many constructive comments and suggestions, they were not asked to endorse the conclusions or recommendations, nor did they see the final draft of the report before its release. The review of this report was overseen by Alton D. Slay, Warrenton, Virginia. Appointed by the National Research Council, he was responsible for making certain that an independent examination of this report was carried out in accordance with institutional procedures and that all review comments were carefully considered. Responsibility for the final content of this report rests entirely with the authoring panel and the institution.

Contents

Summary

The National Institute of Standards and Technology's (NIST's) Material Measurement Laboratory (MML) is the nation's reference laboratory for measurements in the chemical, biological, and materials sciences and engineering. Staff of the MML develop state-of-the-art measurement techniques and conduct fundamental research related to measuring the composition, structure, and properties of substances. Tools that include reference materials, data, and measurement services are developed to support industries that range from transportation to biotechnology and to address problems such as climate change, environmental sciences, renewable energy, health care, infrastructure, food safety and nutrition, and forensics.

At the request of the Director of NIST, the National Research Council formed the Panel on Review of the Material Measurement Laboratory at the National Institute of Standards and Technology and established the following statement of task for the panel:

> The 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 attend an orientation session at the NIST facility, will review technical reports and technical program descriptions prepared by NIST staff, and will visit the facilities of the NIST laboratory. Visits 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 in a closed session panel meeting and will prepare a report summarizing its assessment findings.

The Director of NIST requested that the panel focus its assessment on the following factors:

1. Assess the organization's technical programs.
   - How does the quality of the research compare to similar world class research in the technical program areas?
   - Is the quality of the technical programs adequate for the organization to reach its stated technical objectives? How could it be improved?
2. Assess the portfolio of scientific expertise within the organization.
   - Does the organization have world class scientific expertise in the areas of the organization's mission and program objectives? If not, what areas should be improved?
   - How well does the organization's scientific expertise support the organization's technical programs and the organization's ability to achieve its stated objectives?
3. Assess the adequacy of the organization's facilities, equipment, and human resources.
   - How well do the facilities, equipment, and human resources support the organization's technical programs and its ability to achieve its stated objectives? How could they be improved?
4. Assess the effectiveness by which the organization disseminates its program outputs.
   - How well are the organization's research programs driven by stakeholder needs?

- How effective are the technology transfer mechanisms used by the organization? Are these mechanisms sufficiently comprehensive?
- How well is the organization monitoring stakeholder use and impact of program outputs? How could this be improved?

The MML was formed in 2011 by combining the former Chemical Science and Technology Laboratory, the Materials Science and Engineering Laboratory, and the portion of Technology Services responsible for production, packaging, and sales of NIST reference materials and reference data products. A subsequent reorganization within the MML in 2012 produced six technical divisions (down from 10) and two offices. The two offices manage programs related to NIST Standard Reference Materials and NIST Data Products.

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 creation of knowledge.

The Materials Science and Engineering Division (MSED) provides the measurement science, standards, technology, and data required to support the nation's need to design, develop, manufacture, and use materials with the intent of advancing technology and facilitating manufacturing in industrial sectors such as energy, electronics, transportation, and the environment. The Materials Measurement Science Division (MMSD) develops state-of-the-art instrumentation, analytical methods, models, and software to accurately and precisely measure materials properties, structure, and composition over a wide range of length and time scales for applications such as public safety, forensics, advanced materials characterization, homeland security, and nanotechnology. The Biomolecular Measurement Division (BMD) develops measurement science and standards for macromolecules such as proteins, nucleic acids, carbohydrates, lipids, and metabolites with applications to biopharmaceuticals, DNA forensics, biomedical and bioscience research, and health care.

The Biosystems and Biomaterials Division (BBD) quantifies characteristics of complex biological systems, materials, and processes, from the nanoscale to the macroscale, with the intent of fostering innovation in biomedicine and health care, manufacturing, food safety, environmental health, and national security. The Chemical Sciences Division (CSD) focuses on chemical composition and the chemical structure of gases, organic, and inorganic species and in the measurement of a wide variety of chemical properties and processes, including chemical reactivity and mechanisms, and thermochemical properties. The Applied Chemicals and Materials Division (ACMD) examines the thermophysical and mechanical properties of chemicals and materials, analyzes the reliability and performance of materials and structures, and creates information systems for chemical and materials engineering, with the intent of fostering innovation and confidence in the nation's physical and energy infrastructures, enabling advances in chemical manufacturing and in electronics, and promoting sustainability.

The offices have much more clearly defined functions. The MML Laboratory Office houses the MML's executive leadership (director, deputy director, and executive officer), scientific advisor detailees from the divisions, technical program directors, administrative professionals, and specialists for the functions of safety, communications, grants and contracts, information technology, and human subject protections. The Laboratory Office leads strategic planning, solicits and funds exploratory research, coordinates cross-division scientific programs and the MML's response to national initiatives, and directs top-level communications with stakeholders and the public. The Office for Reference Materials (ORM) provides business, administrative, product, and technical support for the NIST standard reference materials (SRM) program. This includes the infrastructure to produce, package, inventory, and market SRM products and then sell them to customers worldwide. The Office of Data and Informatics (ODI), formed in 2014, will provide the capacity to handle large and information-rich data sources and transform such data into products, such as NIST standard reference data, that can be reliably and broadly shared.

KEY FINDINGS AND RECOMMENDATIONS

Several common themes emerged across the assessments of the MML divisions. Traditional endeavors at NIST prior to the formation of the MML focused on research to improve measurements and development of standard reference materials and data. The work was performed by small groups in divisions stovepiped by scientific discipline. This type of traditional endeavor continues, but now MML scientists and engineers are expected to interact across disciplinary boundaries and participate in large-scale initiatives that require interdisciplinary collaboration within NIST and across the nation, including increased collaborations with academic, industrial, and other government organizations. The MML is continually refining methods for expanding, coordinating, and improving the efficiency of these interactions. The research-oriented staff generally find this change exciting and enabling, but staff whose primary function has been supporting the production of standard reference materials are, in many cases, unclear about their value in the new organization. It is important that the MML respond to the perceptions of staff that there is a need for improved communication of strategic plans at the laboratory and division levels and of the metrics by which successful performance is judged, and that staff desire increased empowerment with respect to the formulation of plans.

The general caliber of technical expertise is competitive with the best large research institutions in the country, but the products generated are generally more varied, because standard reference data, materials, and methods are just as important at the MML as seminal publications or patents.

The high-quality technical work at the MML, in both traditional activities (supporting the development of standards, standard reference materials, and standard reference data) and nontraditional activities (performing research), supported by an excellent equipment infrastructure, is enabling the MML to meet its technical goals. However, the MML is in high demand by external stakeholders, its relevant technologies are leading-edge and dynamically changing, and there is competition for individuals with the expertise required of its staff. The MML therefore faces challenges with respect to achieving an effective balance between maintaining its success in ongoing efforts and initiating new ones that represent appropriate investment of MML resources in niches that will produce the best impact; appropriately allocating the resources of its staff, who are stretched thin in several areas; arranging for staff travel to and participation in activities that maintain and enrich their expertise; maintaining a proper ratio of scientists to supporting technicians; devising succession plans in anticipation of staff who will leave; maintaining an equipment infrastructure by applying make/buy/borrow/share strategies that provide state-of-the-art capabilities within cost constraints; and ensuring that the mission priorities of MML scientists and NIST administrative and legal staffs are aligned with respect to purchasing of equipment and other resources.

MML staff participate in many standards organizations and other professional organizations, and research staff publish papers in peer-reviewed journals. The MML disseminates its many products broadly and has increasing opportunities to expand its dissemination and outreach activities through improved Internet communications.

The findings and recommendations below address key elements in common themes that focus primarily on opportunities to increase the productivity of the MML as a highly valuable and targeted national resource with the potential to play an even greater role in U.S. innovation and competitiveness and to provide an even more broadly based inventory of metrics for use by industry and regulatory agencies.

The MML continues outstanding technical performance in areas related to NIST's traditional endeavors—that is, producing reference materials and supporting the development of international standards. In some cases, the groups in the MML have reached their capacity to support production of reference materials. It is critical for national innovation and industrial competitiveness that leadership in standards development and production of reference materials be supported by first-rate staff and state-of-the-art equipment.

Recommendation 1. The Material Measurement Laboratory should develop a strategy, with significant input from stakeholders, especially industry, to determine which standard reference materials (SRMs) should be terminated, continued, or added. Succession planning for technical staff and project leadership should be carefully addressed to make sure that the capabilities and corporate knowledge pertaining to SRMs do not erode over time. Total manpower and the balance between technicians and Ph.D. staff, financial allocations, pursuit of intellectual property to induce industrial production of SRMs, and other aspects of the process of standards production should be included in the strategic evaluation.

The MML is developing reference data and materials to support less well established industries, including standards for biological materials, nanomaterials, and advanced materials-based products. MML staff are working hard to establish and maintain relationships with relevant industrial and regulatory stakeholders. The identification of which standards or measurement technologies will expedite the critical paths for processing and validation is very difficult. The role of area-specific project coordinators to funnel external queries to the appropriate NIST expert is proving extremely useful. Personnel exchanges with industry would be very useful: MML staff would better understand the development-to-product process and industrial partners could provide input for standards selection. For example, industry fellows could spend time at the MML, and MML staff could spend short sabbaticals learning industrial production processes.

Recommendation 2. The Material Measurement Laboratory (MML) should make much more apparent the focal points for channeling external interactions. The MML should increase the number of project coordinators to funnel external queries to the appropriate NIST expert. The MML should ensure that its portion of the NIST website is updated to market MML capabilities and activities more effectively to potential users of standard methods and materials. The MML should develop additional mechanisms to increase its interactions with industry.

The MML is starting new research initiatives and programs to be responsive to national mandates. These initiatives bring researchers together across MML divisions, across NIST, and externally, with the result that MML staff are very aware of needs and trends for the future. The MML has named technical program directors to manage cross-cutting initiatives across division boundaries. However, at the group level, the near-term objectives and expected deliverables are unevenly defined and the quality of the research is highly variable.

Recommendation 3. The Material Measurement Laboratory should perform technical assessments of research projects at the group, division, and laboratory levels to evaluate the balance between productive existing efforts and new initiatives, to ensure a balance that supports the Material Measurement Laboratory mission, is consistent with available resources, and clearly states the objectives and expected products to all participants.

The Office of Data and Informatics (ODI) has recently been established, and its director has been hired. The ODI will play an important role in support of the Materials Genome Initiative (MGI). However, other MML projects and initiatives are producing highly complex data and need to extract meaningful information from that data. Resources capable of manipulating complex data, data mining to produce knowledge, and disseminating the findings are needed across the MML. The reorganization of the MML has provided opportunities for increased collaborations. One example of leveraging external collaboration is the placement of MML staff at Stanford University to develop biological measurement science, where interactions with faculty and students is a win-win experience for both MML and Stanford.

Recommendation 4. The Material Measurement Laboratory should provide the resources required by the Office of Data and Informatics (ODI) as rapidly as possible. The Material Measurement Laboratory (MML) should integrate the ODI into activities across the MML, especially with any divisions producing information on biological/organic systems. To the extent possible, the MML should leverage outside collaborations while building its own capacity; it should consider using the satellite facility at Stanford as a beachhead to strengthen such connections.

The staff is empowered by the continuity of funding. They are enthusiastic about the opportunity to contribute to national innovation and competitiveness by producing better measurement methods and standards. Staff reported that productivity is clearly hampered by slow responses and multiple levels of administrative oversight external to the MML, especially in the areas of contracting for purchases of supplies and equipment and for legal approvals for industry interactions, work for other government agencies, and use of clinical materials. Achieving the mission of the MML suffers when the controlling priority is compliance with legal and contracting procedural stipulations; both mission accomplishment and compliance should be possible if the priorities are rationally balanced.

Recommendation 5. The mission priorities of Material Measurement Laboratory (MML) scientists and NIST administrative and legal staffs should be aligned. The MML should work to ensure that (a) its staff scientists have simplified training in contracting procedures so they can provide the necessary information at the beginning of a procurement process, and so contracting staff can see how they help the MML to achieve its technical mission; (b) unnecessary legal review and rereview is curtailed by bringing the processes into compliance with standards in other government laboratories and by delegating approval authority; and (c) standard times for review are established to manage MML staff expectations and planning.

The recent reorganization of NIST and the MML has brought the research and standards efforts into much closer contact, in many cases resulting in staff members participating in both endeavors. Therefore, the research is more clearly targeted at producing better measurement systems that will facilitate manufacturing and quality control. Nonetheless, the melding of the standards and research cultures is not without challenges. Some MML staff expressed concerns about the management's perceptions of relative values of traditional activities versus newer research and development activities. Personnel management is uneven. The demonstration project process for personnel evaluation is generally good but needs to be improved. It is administered in different ways in different divisions, and an unacceptable number of supervisors are perceived by staff as ineffective in motivating staff or fostering career development.

Recommendation 6. The Material Measurement Laboratory (MML) should ensure that at the project level the objectives and interrelationship between research and standards development are clearly stated and that supervisors at all levels make clear that both research and standards products/metrics are considered important elements of personnel evaluation, resource allocation, and intellectual regard. The MML should enhance understanding of the performance expectations by providing to all staff annual tutorials covering expectations and metrics for productivity and impact. The MML should establish clear and uniform approaches for creating individual performance plans and reviews; should ensure that reviews are administered using the same process; and should provide supervisor training for all supervisors who have not already taken such training.

1

The Charge to the Panel and the Assessment Process

At the request of the National Institute of Standards and Technology, the National Research Council has, since 1959, annually assembled panels of experts from academia, industry, medicine, and other scientific and engineering environments to assess the quality and effectiveness of the NIST measurements and standards laboratories, of which there are now seven,[1] as well as the adequacy of the laboratories' resources.

At the request of the Director of NIST, in 2013 the National Research Council formed the Panel on Review of the Material Measurement Laboratory at the National Institute of Standards and Technology and established the following statement of task for the panel:

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3. Assess the adequacy of the organization's facilities, equipment, and human resources.
   - How well do the facilities, equipment, and human resources support the organization's technical programs and its ability to achieve its state objectives? How could they be improved?

[1] The seven NIST laboratories are the Engineering Laboratory, the Physical Measurement Laboratory, the Information Technology Laboratory, the Material Measurement Laboratory, the Communication Technology Laboratory, the Center for Nanoscale Science and Technology, and the NIST Center for Neutron Research.

4. Assess the effectiveness by which the organization disseminates its program outputs.
    - How well are the organization's research programs driven by stakeholder needs?
    - How effective are the technology transfer mechanisms used by the organization? Are these mechanisms sufficiently comprehensive?
    - How well is the organization monitoring stakeholder use and impact of program outputs? How could this be improved?

The context of this technical assessment is the mission of NIST, which is to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve the quality of life. The NIST laboratories conduct research that anticipates future metrology and standards needs, enables new scientific and technological advances, and improves and refines existing measurement methods and services.

In order to accomplish the assessment, the NRC assembled a panel of 19 volunteers whose expertise is in the same areas as the work performed by the MML staff.[2]

In April 2014, most of the panel members attended one of two orientation sessions provided at the NIST facility in Maryland. They attended interactive presentations by the NIST Director, the Director of the NIST Program Office, and MML management and staff, and were given tours of the NIST facility.

The entire panel assembled for a day and a half at the NIST facilities in Gaithersburg, Maryland, on June 17-19, 2014, during which time it heard welcoming remarks from the NIST Director's representative and an overview presentation by MML management. Six individual division review teams separately attended division-level presentations and visited the laboratories of the MML divisions: Applied Chemicals and Materials Division, Biomolecular Measurement Division, Biosystems and Biomaterials Division, Chemical Sciences Division, Materials Measurement Science Division, and Materials Science and Engineering Division. Only the Applied Chemicals and Materials team visited the Boulder, Colorado, facility. The panel also met in a closed session to deliberate on its findings and to begin drafting this assessment report.

The approach of the panel to the assessment relied on the experience, technical knowledge, and expertise of its members, whose backgrounds were carefully matched to the technical areas of MML activities. The panel reviewed selected examples of the technical research covered by the MML; because of time constraints, it was not possible to review the MML programs and projects exhaustively. The examples reviewed by the panel were selected by the MML. The panel's goal was to identify and report salient examples of accomplishments and opportunities for further improvement with respect to the following: the quality of the technical programs at the MML; the portfolio of scientific expertise within the laboratory; the adequacy of the laboratory's facilities, equipment, and human resources; and the effectiveness with which the MML disseminates its program outputs. The examples were intended collectively to portray an overall impression of the laboratory, while providing useful suggestions specific to projects and programs that the panel examined. The panel applied a largely qualitative rather than a quantitative approach to the assessment, although it is possible that future assessments will be informed by various analytical methods that can be applied.

The comments in this report are not intended to address each program within the MML exhaustively. Instead, the report identifies key issues. Given the necessarily nonexhaustive nature of the review process, the omission of any particular MML program or project should not be interpreted as a negative reflection on the omitted program or project.

[2] See http://www.nist.gov/mml/ for more information on Material Measurement Laboratory programs, accessed July 15, 2014.

2

Applied Chemicals and Materials Division

The Applied Chemicals and Materials Division (ACMD) consists of 105 staff, who are located in Boulder, Colorado. The ACMD was formed in October 2012 as part of the reorganization of the MML. The reorganization merged the Thermophysical Properties Division (TPD) with the Materials Reliability Division (MRD). These former divisions had very different characters and management styles, which have yet to be completely reconciled. ACMD management presented the following description of its foci:

> The ACMD provides the measurement science, measurement standards, measurement technology, instrumentation, models and data required to support the nation's needs for design, production, and assessment of chemical and material products. In partnership with the U.S. industry, other government agencies, and other scientific institutions, we provide thermophysical and mechanical properties; assess the reliability and performance of materials and structures; and create data management solutions for chemical and materials engineering, with the intent of fostering innovation and confidence in the nation's physical and energy infrastructures, enabling advances in chemical manufacturing and in electronics, and promoting sustainability.[1]

The ACMD is now organized into a Center (Thermodynamics Research Center) and five groups: Experimental Properties of Fluids, Materials for Biological Environments, Nanoscale Reliability, Structural Materials, and Theory and Modeling of Fluids.

ASSESSMENT OF TECHNICAL PROGRAMS

Accomplishments

Maintaining integrity in everything it does is critical for the ACMD, all of whose programs are built on two critical assets: integrity as an honest broker, with scientific results independent of political, regulatory, and legislative influence; and highest quality equipment and measurement techniques, with the personnel to exploit, maintain, and extend precision measurements.

The commitment to quality is clear and pervasive throughout the ACMD. Management and staff are committed to the quality and precision of measurements. The understanding of the fundamental aspects of the most modern tools and facilities is at the deepest level of detail. The work performed in the ACMD can be broadly classified into two broad types, traditional (supporting the establishment of standards) and nontraditional basic research (focused on measurement science).

All of the traditional work reviewed was excellent—the best or among the best of all such work throughout the world. These projects are long-established and form the core of the ACMD's work. As one example, the Structural Materials Group (SMG) continually provides SRMs, calibration and measurement services, property data, and predictive models to ensure materials reliability for structural applications.

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[1] National Institute of Standards and Technology Material Measurement Laboratory, "2014 National Research Council Assessment of the NIST Material Measurement Laboratory-Read-Ahead Materials," Gaithersburg, Md., June 2014.

The SMG has been engaged for over 60 years in mechanical testing; it has also managed the Charpy SRM program for many decades. Similar examples of best-in-the-world excellence in traditional ACMD projects include the Theory and Modeling of Fluids Group's Reference Fluid Thermodynamic and Transport Properties Database (REFPROP) and the Thermodynamics Research Center (TRC). The TRC has produced a set of data that is the standard around the world. Database utilization is embedded in widely used programs (e.g., ChemKin [chemical kinetics] and ASPEN). The output of these programs supports and enables a variety of research scientists and engineers in both academia and industry.

The nontraditional research projects exhibit a widely varied level in quality, from among the top few worldwide to mid-pack at best. The difference among them lies mainly with the level of innovation and likely scientific impact. All of the projects reviewed utilize or intend to develop the best techniques available. They strive to make highly reliable, precise measurements. In nearly all cases, there was significant industrial interest in each project. All the nontraditional projects are squarely within the NIST mission. The research projects whose work is among the top three in the world are the analytical scanning transmission electron microscopy (TEM) work and the resonance atomic force microscopy (AFM) work (e.g., at the Nanoscale Reliability Group), as well as the nascent work on producing top-quality nanoparticles for a variety of applications, ranging from catalysis to water treatment (e.g., at the Materials for Biological Environments Group). An example of a less innovative project with potential impact is the hydrogen and petrochemical pipeline work at the SMG. This is a traditional NIST specialty area based on high-quality but routine mechanical testing. It has been extended significantly in terms of practical importance recently by the novel importation from the Colorado School of Mines of bacteria reflecting pipeline profiles in order to establish the hydrogen activity at relevant conditions. This is the most reliable practical environment ever created for testing in the world, although otherwise the project is based on standard hydrogen embrittlement/fatigue testing. It is invaluable for industry, but it is not particularly innovative in terms of academic research. The strengths and weaknesses of such an approach are entirely appropriate, reflecting the ACMD's mission.

Two noteworthy projects had strong cross-cutting objectives. The work on the Materials Genome Initiative (MGI) is not yet at a stage where its quality can be adequately assessed. Very important research could be performed in this area by extending to materials science the database methods developed by the MML for chemical systems. The work on laser welding is also not yet at a stage yet where its quality can be adequately assessed, but the connections are being formed in a promising manner. This program is uniquely coupling the NIST laser expertise with that in process monitoring and materials characterization.

The main focus of the SMG's programs is in mechanical testing, failure investigations, laser welding, and microbially induced corrosion of structural materials. Thermogravimetric analyses (TGA) give attention to details down to the thermal inertia of the sample holding pans, which is considered imperceptibly small for most research groups yet is accounted for in the uncertainty analyses done at the TRC. Another example is the REFPROP database, where the characterizations of fuel component properties are the best in the world and have been used to help design cooling passages for supersonic flight engines, in which the fuel is used as a coolant.

Understanding the endothermic capability of fuel components is paramount in successful design. There is even recognition that backlash and yaw in a positioning table will result in a quantifiable offset in repeatability. The quantifying of that offset resulted in the installation of independent positioning lasers, completely avoiding reliance on the mechanism of the positioning table. Knowing that there is very slight drift in TGA measurements due to the thermal cycling of the instrument during experimentation is another important element of the required understanding. Therefore, ACMD staff routinely perform calibration before and after an experimental campaign to quantify the drift and incorporate it into the statistical uncertainty of the measurement.

Opportunities and Challenges

The SMG has several new opportunities to expand the scope of its work in numerous NIST initiatives, including those focused on the hydrogen economy, alternative energy, additive manufacturing, and laser welding. The MGI, a cross-cutting effort, is an important initiative that facilitates the extension of the chemical database technology to materials science.

Currently the quality at the TRC is adequate. However, there is a risk in succession planning. The people are the most valuable resource in the research groups. They understand the equipment and the data that are provided by that equipment down to the greatest level of detail. This is developed through a series of steps ranging from understanding the theory of operation to the physical design to limitations of the systems. These steps are a process in learning, using and assimilating acquired knowledge either first hand or through discussions with experienced team members. If there is not sufficient overlap of recent hires with experienced senior scientists, the groups risk having significant intellectual capital not being completely transferred and leveraged.

Overall Assessment of Technical Programs

The SMG fulfills the ACMD mission of providing industry and other customers with measurement science, standards, and technology in structural materials. Researchers at the TRC have produced a set of data that is considered the standard around the world. The research in nanoscale materials with the Nanoscale Reliability Group emphasizes understanding of the measurement technique and the incipient errors; this research is of excellent quality and comparable to the best research performed internationally. The SMG's research programs directly address the main ACMD mission of providing industry and other customers with measurement science, standards, and technology in the area of structural materials.

PORTFOLIO OF SCIENTIFIC EXPERTISE

The people in the ACMD are its most valuable resource. Their determination and creativity have enabled development of some of the translational techniques for which ACMD is recognized. The participation of ACMD personnel on standards committees is noteworthy.

The scientific experience of the SMG can be easily applied to the new opportunities identified above. Some research may be necessary to understand the new challenges such as those encountered in unusual microstructural development in laser welding or the creation of unusual hydrogen activities in microbially induced corrosion of steels. The TRC has expertise comparable to the best scientists in the world. Also, central to the mission of setting standards is the work done by the Nanoscale Reliability Group, which demonstrated the ability to image nanoparticles of diameter 5 nm to 10 nm using a TEM with energies approaching those of a scanning electron microscope (SEM). This has direct application to catalysis and the rational design of catalytically active material.

Sufficient expertise currently exists to support and execute programs. Both junior and senior staff have expressed frustration with the administrative aspects of their work.

The scientific expertise of the ACMD is adequate to perform the required duties. The scientific expertise of the SMG is adequate for the current work as well as for the new opportunities, which are or can be undertaken by the SMG. Recently, the ACMD has built up capabilities in computational materials science to better understand the initiation of fracture.

ADEQUACY OF FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

In general, the experimental facilities in the ACMD are excellent. They include all of the standard characterization and mechanical property equipment. The SMG possesses a variety of equipment for mechanical testing (deformation, fatigue, and fracture), with extensive strain measurement and temperature capability, corrosion testing at high hydrogen pressures coupled with mechanical testing, and Charpy verification. It also has an excellent metallographic laboratory, a microcryocooler test facility, and acoustic emission calibration equipment. This key equipment is adequate to perform the intended work of the SMG. Three technicians maintain and operate this equipment.

The Precision Imaging Facility at NIST Boulder's Precision Measurement Laboratory is a state-of-the-art facility that includes TEM, SEM, atom probe, helium ion microscope, and focused ion beam (FIB) microscopes. The facility appears to be well-supported and has the appropriate staff to run it efficiently. It has a good balance of support projects and technique development.

There is concern with respect to the equipment needed to develop the capability and technique to measure nanoparticles. Based on the discussions with MML staff, if the Nanoscale Reliability Group had not managed, through great patience and perseverance, to assemble the necessary resources, the group's breakthrough might never have happened. Furthermore, it appears difficult for the group to get an updated apparatus to take the measurement science to the next level. The large investment of time and energy devoted to equipment acquisition seems in this case to have been a constant uphill battle, and there is risk that staff may view taking the project beyond the proof-of-concept stage as not worth the effort to initiate this new idea.

There is also concern about mid-career engineers and scientists—namely, there are a small number of mid-career personnel and an associated issue with keeping them engaged, encouraging them to become champions of new directions, and visualizing a path to promotion. Problems and frustrations with the administrative staff seem to contribute to mid-level career burnout. If not improved, this could turn into a problem with succession planning. There needs to be more attention to attracting, hiring, and retaining mid-career personnel. Federal employee positions generally require U.S. citizenship. To attract the best talent in the engineering and science fields, limiting the pool to U.S. citizens may not be the best policy.

Based on tours, discussions with staff engineers and scientists, and an examination of the precision of some of the data generated, it appears the facilities and equipment are adequate. The engineers and scientists understand the equipment to the point where they can modify it to obtain new ways to measure physical properties (such as the AFM vibration test for hardness).

Attention is needed to improve the interest of early-career engineers and scientists in the more mature fields. In addition it appears that two projects were terminated because there was not enough funding to build a critical mass of research activity. It is encouraging that projects can be stopped if it is not possible to obtain data on the needed quality. The nanoneurotoxicity project is an example where it was not possible to obtain reliable cell cultures to generate data sets.

Some groups are not working in novel, leading-edge fields. They could face the risk of not attracting the highest caliber of next-generation scientists and engineers if resources, communicating the importance of a field, and active recruiting are not provided.

The MML director and the ACMD division chief are well-liked and well-respected, and many staff would welcome interacting with them more, particularly on technical matters. Both are good communicators, are open and honest, and seem to have an intimate knowledge of their staff and projects. They seem to provide balanced support. However, both individuals need assistants to give them more time to interact with subordinates individually. The director and the chief seem to have been instilling a better sense of security following the merger, a laudable achievement. All staff with whom discussions were held were willing to talk freely and to express both positive and negative comments. That there is no fear of retribution for being honest is a strong compliment for management style.

Although not stated explicitly by the staff, the rubric "respect for the professional" could subsume the various comments and impressions expressed by some staff. This overarching area demands improvements; those improvements will not require new resources or major changes and can be accomplished over a few years. Examples of such comments (paraphrased) are these:

- There is insufficient transparent communication about management goals and personnel evaluation processes. Performance review standards sometimes change. ACMD management has not been able to achieve adequate cooperation from support staff, including administrators who configure computer equipment and move office equipment without consulting staff, procurement officers who impose processes that significantly delay procurement times, contractors who do not provide desired items, and legal officers who impose counterproductively lengthy reviews.
- Staff are asked to complete numerous surveys that are conceived by a contractor without consulting the staff to determine meaningful questions, and so participation rates are poor, and a common expectation is that nothing will change in response to survey results.
- Staff do not know the strategic plan for the ACMD. Management decisions seem to lack a known strategic context.
- Staff are not involved in hiring, promotion, or compensation decisions.
- Management practices vary from group to group and in some cases from year to year. Group leaders do not receive management training. There are no commonly understood metrics allowing the performance of one individual or group to be compared with that of others.

In addition, new resources may be allocated to a given project without consulting the research staff. This makes maintaining core resources more difficult and necessitates the siphoning off of resources to support core work. There is a struggle between keeping ongoing activities strong while getting resources for new initiatives.

Discussions with managers and postdoctoral researchers suggested a need to speed up the processes supporting procurement and travel.

Overall, the facilities, equipment, and technician resources available to the ACMD are adequate to perform the division's work in established as well as in emerging areas. ACMD staff reported that the procurement and legal systems lead to extreme frustration of the staff. The ACMD staff indicated that administrative staff do not appear to work well in support of the research staff and technical managers at the ACMD; this may be one factor contributing to turnover for some research staff (five have recently left). Some of them perceive that management does not evince sufficient respect for the professional staff.

One way to improve scientific productivity is to ensure that administrative obstacles are removed for the staff members. This action will send a positive message and keep staff motivated while encouraging others to initiate projects. For example, if the procurement process is streamlined, it will ensure that the staff members are focused on projects instead of burdensome paperwork. The procurement and legal processes could be considered as partnerships between the technical and service organizations, with decisions made according to cost/benefit to NIST.

DISSEMINATION OF OUTPUTS

The ACMD has done an excellent job of disseminating its output in the traditional area. It has developed an extremely strong customer base and reports that these customers appreciate the work done at the ACMD. This overall area was the easiest to recognize and appreciate within the TRC. The team does a very good job of active publication, seminar and conference presentations, and workshop participation. In addition, there is active engagement with regulating organizations such as the Food and Drug Administration (FDA) and the Environmental Protection Agency (EPA) and with standardization entities such as the International Organization for Standardization (ISO), the American National Standards Institute (ANSI), and the American Society for Testing and Materials (ASTM).

The SMG influences codes and standards for testing and designing with structural materials. It has provided eight Charpy SRMs to support the certification of Charpy machines for more than 25 years for manufacturers and users worldwide; it evaluates more than 1,000 machines per year from around the world for compliance with ASTM and ISO standards. It is the leading facility for cryogenic flow meter calibrations. The SMG conducts independent, expert investigations into failures of structural materials. In contrast, the dissemination of output in the research area is average in comparison with other research facilities, including universities and national laboratories.

Impact factors and h-indexes from the Institute for Scientific Information (ISI) allow assessing the impact of journal publications. The use of a persistent chemical identifier helps to more accurately track ACMD data used in embedded programs (e.g., ASPEN, ANSYS). ACMD staff monitor and identify stakeholder use, enabling direct discussions with and feedback from all who use their products. For example, the TRC has a consortium consisting of ASPEN personnel, petrochemical manufacturers, and refinery owners.

One improvement needed is to track the progress of new initiatives assessing the quality, pace of progress, and potential payoffs of research. One way this could be done is to hold an open house periodically, where the research champions present their ideas and describe current progress via webinars. This could serve a dual purpose: helping the champion identify and communicate the salient aspects of the project and alerting the community to upcoming techniques and processes coming out of the ACMD.

The SMG has the opportunity to publish in scientific journals its research results in new areas such as laser welding and microbially induced corrosion.

Overall, the ACMD does an excellent job of disseminating their output in the traditional area. Dissemination of output by the TRC is excellent. The SMG disseminates its work through its influence on codes and standards for testing and designing with structural materials. It is well recognized for providing Charpy SRMs worldwide.

FINDINGS AND RECOMMENDATIONS

In general, the traditional projects (e.g., SRMs and databases) are of excellent quality. These activities are prized by the customers in each area as evidenced by communications, purchases of SRMs, and adoption of standards. Examples include setting standards, providing SRMs, and creating and maintaining databases of the best data available (e.g., REFPROP, TRC).

In many cases, the ACMD is the only organization performing this important work worldwide. However, the ACMD is a changing entity, recently reorganized and with many personnel changes. It is important that traditional areas closely related to standards be maintained in spite of current or looming threats. These threats include difficulty in hiring top talent in traditional areas, perceptions that programs in research areas are favored over programs in the traditional standards areas, and difficulty in articulating a commonly understood plan for balancing the two types of activity.

Recommendation: The Applied Chemicals and Materials Division should maintain the traditional areas closely related to standards. The Applied Chemicals and Materials Division should undertake without delay a strategic planning process that includes involvement by its professional staff and addresses the importance of balancing the traditional work with research work.

The average nontraditional project is solid technically but lacks the innovation commonly associated with top academic research. This is not necessarily a weakness; rather, in many cases it reflects the strong and beneficial connections to the ACMD mission and direct response to the needs of industry. The nontraditional projects need not aspire to world-class quality in the academic sense. However, there are a few projects that would be considered top-notch at any academic institution and that also connect strongly with the traditional work.

Recommendation: The Applied Chemicals and Materials Division should consider the needs of industry and the mission of the Applied Chemicals and Materials Division when planning and assessing the non-traditional projects. The recommended strategic planning process should allow the Applied Chemicals and Materials Division to take advantage of emerging opportunities when they arise.

The ACMD has the highest-quality equipment and measurement capability, with the personnel to maintain and facilitate this quality. The ACMD should maintain these excellent capabilities, and ACMD management should work with MML management to ensure that the new tax on capital does not interfere with the excellence of these capabilities.

To the extent that it is generalizable, some staff's perception of poor institutional respect for the professional is a primary threat to continued technical excellence in the ACMD. The following indicators of this perception were suggested by ACMD staff: salaries are low by comparison with salaries of peers employed elsewhere; top-down management and lack of transparency with respect to strategic planning, funding decisions, and personnel performance criteria contribute to a sense of lack of empowerment; lack of training of group leaders results in inconsistency of management styles and practices; and numerous cumbersome administrative, procurement, and legal practices detract from the focus on scientific and technical work and inhibit opportunities for managers to interact with staff.

Recommendation: Applied Chemicals and Materials Division (ACMD) managers should develop and implement novel and pervasive ways of communicating respect, esteem, and empowerment for their subordinates, as a group (i.e., all professionals) and as individuals (i.e., differentiated by accomplishment). Examples should include easing of some bureaucratic burdens, more personal interaction between staff and management, and increased travel opportunities for best producers. The ACMD should ensure that all of its managers have mandatory management training before assuming management responsibility. The ACMD should provide more time and opportunity for face-to-face technical contact between the scientists and the ACMD chief, with the Material Measurement Laboratory director, and with ACMD managers at all levels.

Major aspects of the management of the ACMD are effective in promoting quality and merit in its technical output. The ACMD chief has instilled an improved sense of security among staff that is a remarkable success in view of past funding uncertainties and the recent reorganization of the ACMD. The chief has an open-door policy but insufficient time to initiate routine informal technical interactions. The chief is widely liked and respected by the ACMD staff as a manager and scientist and is seen as open and honest. These positive results could be reinforced by more visits to group meetings, holding semiannual all-staff meetings at which strategic issues are discussed, and sponsoring informal social events. Such expansion of communication efforts requires time that could be made up for by delegating other responsibilities.

Recommendation: The Applied Chemicals and Materials Division chief should continue and expand the effective communication practices that foster staff morale and productivity.

3

Biomolecular Measurement Division

The objective of the Biomolecular Measurement Division (BMD) is to develop measurement technology, standards, and data to determine the composition, structure, quantity, and function of biomolecules. The work focuses on bioprocessing, applied genetics, mass spectrometry, biomolecular measurement, biomolecular (protein) structure and function, and bio-analytical science. These areas are identified using terminology that is consistent with the terminology used for research areas in systems biology and molecular biology. The actual work being carried out by the BMD appears to be more focused than what is indicated by the groups' titles. Specifically, the BMD, which has 11 staff in its headquarters office and 100 others elsewhere (including 30-35 guest researchers), is divided into projects conducted by five groups.

The Mass Spectrometry Data Center develops mass spectral libraries for small molecules, metabolites, peptides, glycans, and proteins; the Applied Genetics Group develops standards and technology for DNA testing to aid human identification efforts and to support biometric, law enforcement, and clinical applications using genetic information; the Bioanalytical Science Group develops protein-based standard reference materials such as C-reactive protein (CRP) and bovine serum albumin (BSA); the Bioprocess Measurements Group develops measurements for counting and sizing biological particles (protein aggregation and preparation of protein particle surrogate materials as SRMs); and the Biomolecular Structure and Function Group performs work in crystallography, neutron scattering, and nuclear magnetic resonance (NMR) to determine the structure of biomolecules (including a monoclonal antibody standard).

The five groups carry out their work on the main campus and at the Institute for Bioscience and Biotechnology Research (IBBR) at Rockville, Maryland. These groups appear to have distinct goals, but at the same time they carry out work on complementary research topics and technical themes directed at the forensics and diagnostics of nucleic acids (DNA), peptides, proteins, and macromolecules in addition to smaller molecules. Characterization of chemical molecules and peptides is the major mission of the Mass Spectrometry Data Center. A significant capability of the BMD is at the IBBR, which carries out work on proteins and macromolecular structures with initiatives in biopharmaceutical measurement and engineering. This work is centered on the facilities in Rockville, including a 900 MHz NMR spectroscopy system housed in the W.M. Keck Structural Biology Laboratories. In addition to fundamental research related to a range of proteins, nucleic acids, and nucleic-acid protein complexes, NMR methods are also used to study protein folding, stability, and interactions in solution in order to develop models, standards, and databases.

The number of people associated with the groups is given in parentheses: Mass Spectrometry Data Center (32), Bioprocess Measurements Group (22), Biomolecular Structure and Function Group (20), Bioanalytical Science Group (13), Applied Genetics Group (12), and the Biomolecular Measurement Division headquarters (11).

Thirty-five percent of the division's researchers and employees consist of guest researchers and 65 percent are federal employees. The budget of the BMD is $23.3 million (fiscal year 2014) with $5.47 million of the $8.86 million biomanufacturing initiative being awarded to the BMD. There are three primary products of the BMD: measurement science and protocols disseminated through scientific publications, standard reference materials and reference data, and spectral libraries.

ASSESSMENT OF TECHNICAL PROGRAMS

Accomplishments

While the biomolecular component of the BMD suggests that the activities of this division focus on measurement science, standards, and data and technology for biomolecules and biomacromolecules. A major component of this division's work also addresses reference data and spectral libraries for smaller compounds (including biologically relevant low-molecular-weight metabolites and peptides) through the Mass Spectrometry Data Center. The center's work is a major component of the BMD's overall effort and has national and international impact for the identification of chemical entities through their mass spectral fingerprints. The center is responsible for NIST-evaluated spectra, together with validated software for spectral matching packaged in a user-compatible visual interface. These products are widely integrated into instrument vendor software systems. The reference database is the world's most widely used mass spectral library and is delivered, together with commercial instruments, through the companies that produce, market, and service mass spectrometers. More than 5,000 new installations of these reference data and software occur each year. The mass spectral library is an important component of standard reference data sales by the MML. The MML accounts for 98 percent of standard reference data sales in NIST. In 2013, 79 percent of MML sales were derived from the mass spectral library.

The work on measurement science, mass spectrometry data, and protocols for forensics involving DNA are major and continuing contributors to the impact of the BMD. Many BMD activities are oriented to understanding the impact of alterations in protein structure that indicate changes in identity, purity, or function, thereby creating the knowledge that will be critical for biomanufacturing or health regulation. This effort involves significant exploratory research and is defining the problems that need to be addressed. The donation of a significant quantity of a humanized monoclonal antibody (mAb) by Medimmune, LLC (now a division of AstraZeneca) has provided material for a wide variety of development efforts focused on protein metrics and models that describe effects of the protein's environment (pH, ionic strength, other proteins, etc.) on structure and function. This focus involves a major effort not only in the BMD, but across the MML, and fosters internal and external collaborations. Discussions with researchers at the IBBR suggested that this mAb is being used as a reference against which the characterization of other proteins may be compared as the BMD advances its capabilities in protein characterization.

The Bioprocess Measurements Group combines expertise in instrumentation science, nanomaterials, and chemical and physical characterization of surfaces, sensor materials, and biological molecules to address measurement needs relevant to biological industrial processes.

The Biomolecular Structure and Function Group is located primarily on the main Gaithersburg campus, with another facility near Rockville and a University of Maryland facility nearby. These locations enhance the group's collaborations external to the MML, especially with the University of Maryland, industry, and—separately—with the FDA. This group is focused on measurement of disease pathways, vaccines, protein therapeutics, and biomarkers for diagnostics. The studies on proteins in the new 900 MHz NMR, compared to those produced by more common instruments, will inform more efficient use of the latter for bioprocess analysis. The studies expand the study of proteins to include RNA, lipids, and glycans. Cutting-edge instrumentation is used to develop measurement technology to extract information on molecular function, structure, and responses to molecular interactions and changes in the environment (e.g., temperature, humidity, pH, and sample matrix). These types of data are critical for the bioprocessing industry and biotherapeutic applications.

The Bioanalytical Science Group is developing reference materials based primarily on proteins, including reference standards for bovine serum albumin, C-reactive protein, and an IgG mAb. The technologies used to characterize these materials are state of the art, and the staff are very aware of the need to distinguish properties relevant to function in addition to those indicative of purity and structure. The data obtained from characterization of the NIST mAb will be published in an American Chemical Society book by the end of 2014 and will be the most exhaustive analysis of a single protein performed to date, with more than 60 collaborating partners involved.

The Applied Genetics Group validates instruments and methods used for forensic genetics. It provides DNA profiling reference materials that are used to ensure that forensic laboratories are generating accurate and reliable results. The group has produced a DNA reference material for clinical diagnostic laboratories to ensure the accuracy and comparability of test results for Huntington's disease. It is expanding this program into other clinical areas. An extensive sequencing program is testing methods and instruments for rapid polymerase chain reaction (PCR) technologies and rapid gene sequencing. This program has produced a variety of standard reference materials, methods, and data.

Review of the accomplishments of the five groups shows a range of valuable products for clinical diagnostics; genetics; viral genetics; pharmaceutical products; environmental, food, and forensic analysis; biosensor development; structural characterization of large molecules (particularly proteins); and the previously mentioned mass spectrometry database. The achievements are significant and impact the pharmaceutical, clinical diagnostic, chemical, law enforcement, and biopharmaceutical sectors (Table 3.1). Some of the more recently initiated work in structure/function studies for protein therapeutics and biologics needs more time to develop, given the rapidly changing character of the biotechnology industry and the demands for new products that address human diseases in a cost-effective manner. Achievements and impact will likely evolve as the capabilities and focus of IBBR activities continue to develop and data from this facility become available, at first internally in the MML and then more widely to the biopharmaceutical industry.

Opportunities and Challenges

The research on protein structure and modifications that impact function is needed, but the challenge is to focus the research so that it complements related work supported by industry as well as the $25+ billion budget of the National Institutes of Health (NIH). There is recognition at the division and group levels that such interactions are important, but a specific approach to how the needed connections will be made and used to inform the work of the BMD is less clear.

TABLE 3.1 Biomolecular Measurement Division: Summary of Activities and Achievements

Group	Capability	Impact
Mass spectrometry data	Mass spectrometry of chemicals, proteins, peptides, glycans, metabolites, and lipids	NIST/EPA/NIH mass spectral library broadly used in industry
Bioprocess measurements	Protein particles, interface, and characteristics; sensors	Microfabricated devices, protein stability data
Biomolecular structure and function	Macromolecular structure/function	IBBR, biosensors, protein therapeutics
Bioanalytical science	Small molecule/biomolecules, Standard reference material development, LC/MS	BSA (protein) standard reference materials, protein metrology
Applied genetics	DNA typing, sequencing, multiplex PCR, qPCR, DNA mixture interpretation	Forensic and clinical genetics, DNA fingerprinting, DNA identification instruments

NOTE: LC/MS, liquid chromatography/mass spectrometry.

As an example of one standards development effort for biomanufacturing, the Bioprocess Measurements Group is examining measurement of protein particles and aggregate formation, leading to the preparation of a nanostructured particle that has a shape similar to that of a protein aggregate. While this is an impressive technical achievement, it is not clear that the scientists have given thought to the other factors that need to be considered, because shape alone is not sufficient to define a protein aggregate. Other factors that need to be considered include amino acid sequence, cross-links formed, solution pH, and temperature history.

A significant issue that the BMD would like to pursue is to develop tests for protein potency. How does one relate physicochemical characteristics to protein functionality? This is a very important question whose answer would involve collaboration between the BMD and the Biosystems and Biomaterials Division of MML, and probably some of the other divisions. If the BMD could discover some revealing physical metrics that are reliable indicators of function, expensive tests using cell culture and whole animal systems could be drastically reduced.

The BMD has the opportunity to develop cross-disciplinary culture and to pursue complex issues faced by the growing biomanufacturing sector in the United States. This sector may expect process-specific standard reference data and materials, while the BMD will need to be able to prepare materials that have a broader utility across the industry. If this is the case, strategic allocation of capabilities and resources within the BMD, and more broadly the MML, will need to be achieved in the coming years. A team approach with specific or allocated tasks for each team member will need to be set forth and managed.

Overall Assessment of Technical Programs

Overall, the BMD program includes strong individual efforts, but the complexity of biomolecules requires that a more integrated approach be defined. The need to understand information relevant to function as well as structure needs to stay in the forefront as future priorities for programs are established. An overall assessment of the BMD’s technical programs shows programs consistent with the mission of NIST and the MML. The BMD is addressing biotechnology for forensics and biomanufacturing and is part of the initiative in big data.

The BMD groups show strong individual efforts, while at the same time providing complementary expertise among the programs pursued by the five groups (refer to Table 3.1). All of the groups show productivity in publishing (roughly one paper per person per year) and align with the BMD’s goal of disseminating measurement science and protocols through scientific publications. In addition, the groups also provide either reference data or reference standards to the industry, as summarized in Table 3.2.

At the same time, the complexity of protein structure and function and the classification of some of the proteins in terms of their production process (rather than just their composition) add complexity to the approaches that need to be developed. Unlike chemical or peptide reference data or samples, protein data need to reflect differences in protein glycosylation patterns, protein cross-linking, refolding patterns, and post translation modification—that is, changes that occur after the cell expresses or releases the newly formed protein.

The technical programs, and particularly the intragroup dynamics, appear to be good. However, the goals and the products to be generated as a consequence of these goals still need to be defined in some cases. In the case of chemical molecules, the goals and framework for achieving the goals are clear, and the instrumentation and analytical methods needed to carry out the measurements are available and readily carried out.

TABLE 3.2 Standard Reference Materials Prepared by the BMD

SRM	Description
927E	Bovine serum albumin (7% solution)
998	Angiotensin I (human)
2366	Cytomegalovirus (CMV) for DNA
2372	Human DNA quantitation standard
2389A	Amino acids in 0.1 mol/L HCI
2391C	PCR-based DNA profiling
2392	Mitochondrial DNA sequencing
2392-I	Mitochondrial DNA sequencing
2393	CAG repeat length mutation in Huntington's disease
2394	Heteroplasmic mitochondrial DNA mutation detection standard
2396	Oxidative DNA damage mass spec.
2921	Human cardiac troponin complex
8323	Yeast protein extract
8327	Peptide RM for molecular mass
In development	
998 A	Angiotensin I (human)
1989	Ethylene tetrafluoroethylene for particle size distribution and morphology
2365	BK virus for DNA measurements
2366A	Cytomegalovirus (CMV) for DNA measurements
2922	Cardiac troponin I in serum
2924	C-reactive protein solution
2925	Human serum albumin solution
2926	Human insulin-like growth factor 1
3666	Albumin and creatinine in frozen human urine
8313	Digested yeast protein extract
8321	Peptide mixture for proteomics
8671	NIST mAB, humanized IgG1K

The reorganization of the MML was carried out to achieve more formally managed cross-division technical programs and to address cultural, organizational, and management barriers to staff interactions and collaboration across divisions. While strong interdivision collaboration needs to be proactively encouraged, cooperation and collaboration between groups within a division may also need to be encouraged.

The BMD was formed as part of the MML reorganization, and the division is working on enhancing collaborations and cooperative work within the division. A division seminar series was mentioned as a tool to help people get acquainted with the work of others both on an intra- and interdivisional basis. While this is a start, a first impression is that further development of intra-divisional work, particularly between Gaithersburg and Rockville (IBBR), is needed. While the biomanufacturing program has assisted in cross-division collaboration, this cooperation needs to be reinforced and further developed.

Biologic drugs are both a U.S. economic driver and a health care cost issue and may benefit from the establishment of standards. The recent focus of the BMD on biologics, particularly through the IBBR, is appropriate but also complex, in that the molecules to be studied, and for which reference data and/or standards are needed, are also very complex and manufacturer-specific. However, if the BMD is to successfully address this challenge, close cooperation between the Bioanalytical Science, Bioprocess Measurements, Applied Genetics, and Biomolecular Structure and Function groups will be needed to address standards at each step of the research, development, and, ultimately, manufacturing processes: (1) identifying a protein therapeutic candidate; (2) cloning and development of a host organism, (3) cell culture and protein production, (4) protein purification, and (5) formulation and fill.

These steps are part of a complex manufacturing process, where each step may impact the characteristics of the biomacromolecules. The BMD has recognized the inherent challenges, but the groups need to work together to identify where concerted efforts would tap into the unique capabilities of the BMD and the MML to make a difference in reducing costs of biologic drugs through standards that only the MML could provide.

The workshops that the BMD has organized and participated in have addressed topics that will assist in developing strategies for entering new areas of biomanufacturing where standards are needed. Examples of these workshops include a biomanufacturing summit, applications of mass spectrometry for biopharmaceutical manufacture and characterizing biopharmaceuticals in a regulatory setting, and next-generation characterization tools for therapeutic proteins. Overall, these programs and activities represent excellent first steps in defining the role of the BMD in developing standards and meeting the goals of the MML for the next-generation bio-based products.

PORTFOLIO OF SCIENTIFIC EXPERTISE

The scientific staff have made significant accomplishments. There is significant variability in publication output, from easy-to-measure to the more difficult to quantify information and standards provided to industry. Overall the output is respectable when compared to the measure of papers that are published by academic counterparts in related fields. These numbers could be higher, but many of the staff are engaged primarily in exploratory research. However, the value of the work lies in its development of clearly defined standards. One such standard might specify, for example, the forensic accuracy of commercial gene typing instruments, which are much more complex than, for example, the concentration of BSA in solution. While both are important, defining the reliability of an instrument or protocol used in courtroom proceedings is a task that the MML would seem uniquely qualified to do.

The opportunities and challenges in terms of scientific expertise are to integrate the historic strengths of the MML, that is, standard reference materials, with the technologies used to characterize and produce them. This is particularly important in the biotechnology industry, because the products are not as well defined chemically or physically as, for instance, the molecules encountered in metallurgy, organic chemicals, small molecules, pesticides, and other more discrete chemical entities with which the BMD has significant experience. Consequently, a directed effort will be needed to carefully foster expertise relevant to the development of standard measurements for characterization of biomolecules (an example would be the skill required to characterize a monoclonal antibody using 900 MHz NMR).

The portfolio of scientific expertise at the division level has individuals who are outstanding scientists in their area and who work well as members of teams defined by discipline or investigating a specific target material or molecule. As the MML moves into the biotechnology and bioproducts areas, the BMD needs to define the types of measurements and standards the industry will need. These could be diverse, ranging from standards for improving efficiency of manufacturing technologies for biomolecules used in pharmaceuticals, to protocols for improving diagnostics of human or animal diseases or identifying biomarkers indicative of disease. There is the potential for considerable overlap of the activities of the BMD with the activities of other agencies, so goals need to be selected that focus on work that is synergistic with the goals of those other agencies.

ADEQUACY OF FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

The BMD reported many significant accomplishments. The successful projects varied from developing instruments and defining protocols for forensic genomics for personal identification to characterization of complex proteins that define some types of biopharmaceutical molecules. The developments with respect to characterization of proteins may in some cases lag the field with respect to knowledge and protocols already developed in the industry but may in other cases be useful for identifying appropriate measurement techniques and instruments that could give useful data in the absence of extensive and expensive facilities like those at the BMD. The group with the most internationally recognized accomplishments is the one that operates in the area of mass spectrometry—this mature team is large and highly focused.

The BMD has tremendous intellectual capital, state-of-the-art facilities, and a mandate to develop standards and protocols for materials that are likely to emerge from the continuing and rapid development of biomolecules, including biopharmaceuticals, biopolymers, and specialty bioproducts used as precursors in biochemical manufacture. The challenge will be to apply the limited resources available to the BMD wisely and to target areas that cut across different industries or companies in a way that benefits the industry and, at the same time, is accepted by individual companies as part of their manufacturing technology and regulatory ecosystem. This will require a deep understanding by the BMD of the manufacturing processes that these companies utilize and the ability to propose reference materials and information that would assist them in developing their manufacturing processes. Consequently, the staffing of the BMD needs to reflect this mission, and the division may need to increase their exposure to problems of biomanufacturing in order to carry out targeted work in their mission of biomolecular measurement.

The BMD has excellent facilities and human resources that could have a major impact if they are directed toward specific targets and industry needs that transcend the capabilities of large or small individual companies to address. A survey of these needs by an organization such as the Pharmaceutical Manufacturers' Association (PMA) or one of the committees of the Biotechnology Industry Organization (BIO) may be useful.

DISSEMINATION OF OUTPUTS

In addition to the mass spectrometry database and the widely used albumin standard, the outputs of the BMD include DNA standards, biomarkers, and forensic training.[1] In all these cases, the information that is bundled with the standard reference materials has made a major impact on the industry and the ability to manufacture products (even if by different processes) that have common characteristics, identifiable qualities, and safety. This is a key to the contributions made by the BMD and also to the recognition of the value of the MML in impacting the industry in many but subtle ways. It is important to maintain this combination of data, information, and reference materials.

The provision of standard reference materials, vetted results on new instruments, and assessment of data validity are needed to ensure that industry and law enforcement agencies are able to produce reliable information. The challenge is in developing efficient and effective approaches to obtaining a deep

[1] NIST Material Measurement Laboratory, *Turning Ideas Into Innovations*, Gaithersburg, Md., August 2012.

understanding of biomanufacturing processes, which are often less well defined and at much earlier phases than the mature industries. This knowledge is needed to ensure that dissemination of outputs is carried out in a useful, timely, and accurate manner and that the MML is able to increase the efficiency of innovation and manufacture of bio-based products. The dissemination of web-based products has not realized its potential, and there is plenty of opportunity for improvement.

The analytical focus on biomolecules is yielding important information and opportunities to develop standards. The next step, extraction of knowledge from the data, needs increased attention in terms of how to do it, how to understand it, and how to share it.

FINDINGS AND RECOMMENDATIONS

The recommendations below relate principally to how the goals and metrics of performance are articulated, with emphasis on the importance of maintaining many of the positive aspects of the BMD that make it a unique and valuable resource to the industry.

A BMD strategy integrated with an overall MML strategic plan is needed to clearly map the pathway from current BMD strengths to the development of excellence in applying standard metrics to biomolecules.

Recommendation: The Biomolecular Measurement Division should define a strategy that will specify which biomolecules will be selected to be standards, what information is required about those biomolecules, and how they relate to other molecules that are likely to become important in the emerging industry.

Data acquisition is only the first step in providing standards for the biotechnology area. Developing a focused and integrated plan on data informatics is particularly important for BMD standards efforts.

Recommendation: The Biomolecular Measurement Division should develop a focused and integrated plan on data informatics. Such a plan can be developed in conjunction with a more complete assessment of the future needs of biomanufacturing to drive the selection and dissemination of Biomolecular Measurement Division standards.

The BMD needs a much deeper understanding of biomanufacturing processes, which are often less well defined and in much earlier phases than the mature industries that MML has historically addressed over the past 20 years. This understanding is needed to ensure that appropriate research targets are selected at the MML and that generation and dissemination of outputs to the biomanufacturing industry are carried out in a useful, timely, accurate, and relevant manner.

Recommendation: The Biomolecular Measurement Division (BMD) should extend its industry interactions. In addition to workshops and ad hoc collaborations, they should explore personnel exchanges—for example, by hosting industry fellows at BMD facilities and arranging short sabbaticals for its staff at bioprocessing facilities. The BMD should encourage and support staff members' more frequent attendance at industry-oriented conferences and workshops (as compared to research-oriented meetings).

The BMD is struggling to derive the knowledge to underpin the selection of metrics critical for biomanufactured products. Developing such an understanding is a difficult and very important challenge. The BMD needs more collaborative interactions to achieve this knowledge.

Recommendation: The Biomolecular Measurement Division should undertake a closer working relationship with the National Institutes of Health and the Federal Drug Administration, complemented by industry collaborations, and should use these collaborations during the process of prioritizing its work and ensuring that the data obtained is relevant to measurements that are essential for the field of biomolecules, biotherapeutics, and biosimilars.

Personnel management at the BMD appears uneven and handled with variable effectiveness, resulting in very different expectations, especially among junior staff. Mentoring of postdoctoral researchers tends to be excellent, but mentoring of junior permanent staff is very uneven. Understanding of technical goals, especially those of cross-divisional projects, is limited in some cases. With the exception of their frustration due to contracting and technology transfer administration, most staff are very happy about the working environment. However, it is important that the BMD management communicate the technical strategic plan to all its staff, make supervisory processes transparent, and remove, to the extent possible, unnecessary roadblocks to purchasing and collaboration. These actions are needed if the excellent morale, can-do attitude, and commitment to excellence in measurement results are to be maintained within the BMD.

Recommendation: The Biomolecular Measurement Division management should communicate the technical strategic plan to its entire staff, make supervisory processes transparent to staff, and remove, to the extent possible, unnecessary roadblocks to purchasing and collaboration.

4

Biosystems and Biomaterials Division

The mission of the Biosystems and Biomaterials Division (BBD) is to address the nation's needs for measurement science, standards, data, methods and technology in the quantification of complex biological systems and materials and processes. The BBD partners with U.S. industry, government agencies, and scientific institutions to develop the infrastructure supporting quantitative biology and biomaterial measurements, with the intent of fostering innovation in health care, manufacturing, food safety, environmental health, and national security.[1] The BBD consists of 114 staff members in four organizational groups that support 15 technological application teams.

The Bioassay Methods Group addresses areas such as flow cytometry, reference gene assays, and cancer biomarker standards for cancer diagnosis and therapeutics.

The Biomaterials Group includes application teams in cell materials interactions, three-dimensional (3-D) tissue engineering scaffold material characterization, and protein stabilization. The Biomaterials Group's imaging and spectroscopy technologies focus area includes application teams in benchmarking and calibrations, broadband coherent anti-Stokes Raman Scattering (BCARS) microscopy, live single-cell analysis, and flow cytometry.

The Cell Systems Science Group includes application teams in cell-based therapies; microscopy benchmarking; synthetic biology; cell line identification; nanotechnology environment, health, and safety (NanoEHS); and measurements for assessing nanoparticle effects on biological systems.

The Genome Scale Measurements Group includes application teams in clinical diagnostics, synthetic biology, and microbial identification.

The BBD research activities focus on providing validated methods and measurements, technologies, and data and standards to advance the understanding of complex biological systems and biomaterials through characterization and quantification. This is accomplished by working from the molecular to supramolecular scale, examining the complexity of communication between cells and cell interactions with materials, developing tools to address the challenges of measuring biological functions, and enabling biology to become more of an information science for health, predisease, and disease.

ASSESSMENT OF TECHNICAL PROGRAMS

Accomplishments

Bioassay Methods Group

There are four major programs within the Bioassay Methods Group (BMG): spectroscopy standards, biomarker quantification, flow cytometry, and engineering biology. Staff expertise is very diverse and broad. The staff have supported the development of wavelength, photometric and stray light standards for ultraviolet, visible, and near infrared (UV-Vis-NIR), Raman, and fluorescence

[1] NIST Material Measurement Laboratory, "2014 National Research Council Assessment of the NIST Material Measurement Laboratory: Read-Ahead Materials," Gaithersburg, Md., June 2014.

spectroscopies, developing 20 SRMs and 200 recalibrations of photometric standards every year; established traceability in flow cytometry with fluorophore solutions and calibrated beads; developed reference materials and protocols for benchmarking fluorescence microscopes; developed the first international reference standard for CD4+ cell counting for HIV/AIDS monitoring[2]; developed an equivalent reference fluorophore unit for microsphere calibration materials and directed a fluorescence value assignment training program to bead manufacturers with the International Society for Advancement of Cytometry; established assays for HER2 using quantitative PCR and digital PCR; established reference gene assays on chromosomes that are not commonly mutated in cancer; and started high-throughput DNA sequencing for cancer genes on the DNA standards.

The BMG has generated assay, data handling, and results interpretation schemes for assessing the characteristics of mitochondrial DNA as a potential prostate cancer biomarker using qPCR assay and first reported that a 3.4 kilobase mitochondrial DNA deletion and an increase in mitochondrial DNA copy number, as potential prostate cancer biomarkers, can be detected in urine and serum.

The group developed an internal fluorescence reference method to allow quantitative comparison of expression of markers for pluripotency and patented the method for potential development as a kit to enable widespread application; in collaboration with NIST's Information Technology Laboratory, developed methods for automatically scoring stem cell colonies for their pluripotent character; developed a bioinformatics approach to identify potential short tandem repeat (STR) markers and analytical measurements to measure multiplex STR markers; developed an African green monkey cell line multiplex STR assay; developed a mouse multiplex STR assay and applied for a U.S. patent (the assay was licensed and is being commercialized by DNA Diagnostics Inc.); began development of an STR multiplex assay for Chinese hamster ovary (CHO) and rat cell lines; used cause-and-effect diagrams to identify sources of variability in an MTS nano-cytotoxicity assay protocol, leading to redesign of the protocol to include seven additional control experiments; designed and executed an interlaboratory (including measurement institutes in the European Union, Korea, Switzerland, Thailand, and the United States) comparison study of the MTS cell viability assay as a nano-cytotoxicity assay; and used advanced statistical analysis techniques to quantify nano-cytotoxicity assay variability and to identify steps in the protocol that are likely contributing to variability in the assay result.

The Bioassay Methods Group has produced 18 unique SRMs for ultraviolet-visible, near infrared, and Raman spectroscopy, fluorescence, and flow cytometry techniques—SRM sales have been approximately 170 units per year; developed methods and standards to support cell line authentication; developed the equivalent reference fluorophore calibration approach that has been accepted by the flow cytometry community; and with two other national metrology institutes developed the first international reference cell standard for CD4+ cell counting for HIV/AIDS monitoring (WHO/BS/10.2153).

Biomaterials Group

In 2001 the work of the Biomaterials Group was expanded beyond dental research to include standards and advanced technologies for emerging diagnostics and therapies. The group is working in the areas of dental materials, 3-D scaffolds for tissue engineering, broadband coherent anti-Stokes Raman scattering (BCARS), and protein preservation.

Its accomplishments include new materials, theories, and models; measurement technologies and standards aimed at assuring safety and performance of devices; a large research portfolio that includes tissue engineering, cell–material interactions, stabilities of protein therapeutics (drug delivery), biomineralization, smart materials, antimicrobial materials, and measurement of complex structure–property relationships of dental and biomaterials development of international documentary standards; a validated, patented instrument for simultaneous measurement of polymerization kinetics, reaction

[2] World Health Organization, "Requests to Initiate New WHO Reference Material Projects," WHO BS/10.2153, Geneva, Switzerland, June 22, 2010.

exotherm, and polymerization stress for photopolymerized composites; a long-term collaboration (since the 1930s) with the American Dental Association (ADA), which now represents over 150,000 dentists, to provide assurance for the program's strategic directions; a tabletop steady-state fluorescence instrument that could easily be used in a biopharmaceutical laboratory to provide relevant nanosecond dynamics; four NIST reference materials for measuring porosity of and cell proliferation on scaffolds; combinatorial cassettes as high-throughput, systematic in vivo testing platforms to increase measurement confidence and reduce the number of animals needed for testing; 3-D image analysis methods for quantitative descriptors of cell and scaffold shape metrics; and the largest study of 3-D stem cell morphology, involving 1,500 z-stacks of stem cells and 1 TB of data, to determine the role of cell shape in biological response.

Major research findings from the Biomaterials Group have been published in 17 peer-reviewed papers. Since October 2012, 11 invited presentations have been delivered and one patent application has been filed. The group has developed new methods using coherent Raman effects (BCARS) to acquire vibrational spectroscopic image data at ever-shorter acquisition times—the group demonstrated acquisition of spectral images from live cells at 50 ms/pixel, at least 100 times faster than spontaneous Raman, and in 2013 was the first laboratory to demonstrate spectral image acquisition from tissues at 3.5 ms/pixel.

Cell Systems Science Group

The Cell Systems Science Group has demonstrated SPR imaging through a high numerical aperture (NA) microscope objective and the novel use of a digital light projector to achieve near diffraction limited in spatial resolution (representing a 10-fold improvement), allowing for unprecedented visualization and quantitation of subcellular features, including measurement of protein density in focal adhesions. It also developed a prototype standard reference image database (SRD 159) to discover and disseminate the image data—the discoverability of the data is made possible through annotation with an advanced rule- and root-based terminology technology designed to enable federated database storage.

The group addresses applications in emerging stem cell technologies, organismal scale metrology, and nanotoxicity. It focuses on the cell as a system and tools that measure and characterize system properties in basic biomedical research, biomanufacturing, and regenerative medicine, and on other applications that depend on understanding and predicting complex cellular activities. It assesses sources of variability in a protocol using experimental design and control experiments. The group also participates in standards committees to facilitate dissemination and knowledge transfer of good measurement practice and development tools that facilitate validating cellular populations as reagents.

Team scientists develop measurement assurance strategies for cell biology that include cell-based assays for nano-cytotoxicity measurements and measurement needs in the cell therapy community. The Cell Systems Science Group conducts four programs: assurance and comparability in cellular measurements, tools for terminology development for annotating biological data, assurance in organism scale measurements, and live cell imaging and modeling.

The group developed a bioinformatics approach to identifying potential STR markers and analytical measurements of multiplex STR markers; developed African green monkey and mouse cell line multiplex STR assays; formed a cooperative research and development agreement (CRADA) with DNA Diagnostics, Inc., to jointly work on the mouse assay (DNA Diagnostics is planning to develop a database of profiles of mouse cell lines to facilitate identification, and other companies have expressed interest); supported development of an ANSI/ATCC consensus standard to identify cell lines at the species level using DNA bar-coding; completed design and construction of a *Caenorhabditis elegans* laboratory; initiated adaptation of the ISO *C. elegans* toxicity assay to a *C. elegans* nano-cytotoxicity assay for a document for the Organization for Economic Cooperation and Development; collaborated with the Alliance for Regenerative Medicine on white papers on measurements for cell therapy products; through the ASTM F04 and ISO 276 committees, worked with the community to identify reference materials and standards needed for cell therapies; and collaborated with Lonza Group Ltd. on statistically evaluating the accuracy of cell enumeration by automated NucleoCounter and manual hemocytometer methods.

Genome Scale Measurements Group

The Genome Scale Measurements Group has facilities in Gaithersburg, Maryland, and at Stanford University in Palo Alto, California. It is organized to develop and disseminate new measurement science, reference materials, data, and methods for genomics. The group works closely with many stakeholders, such as public–private–academic consortia, the External RNA Controls Consortium, the Genome in a Bottle Consortium, and the Synthetic Biology Standards Consortium. It also works with many of the federal agencies, including the FDA, NIH and its National Cancer Institute (NCI), the Defense Advanced Research Projects Agency (DARPA), and the Department of Homeland Security (DHS).

The Genome Scale Measurement Group's accomplishments include methods for genome scale measurement assurance and sequence certification; DNA library reference materials, data, and methods; reference materials, data, and methods for the External RNA Controls Consortium (ERCC) dashboard. The software package analyzes results from measurements of RNA spike-in experiments to understand technical performance of single-cell transcriptome sequencing.

In 2012, NIST convened the Genome in a Bottle Consortium, a NIST-hosted public–private–academic partnership to develop the metrology infrastructure for widespread adoption of human genome sequencing in research and regulated clinical applications. The Genome Scale Measurements Group worked with Ambion® to develop an accurate set of controls, consulting on the design of the mixes and their quality assurance protocols; it also developed reference materials and methods for the Genome in a Bottle project. The group is planning to develop a refined set of controls as a follow-on product to address new RNA measurement science needs, including small nontranslated RNAs, transcript isoforms, and microRNAs (miRNAs)—this refined set of controls will be established as a rebooting of the ERCC (ERCC 2.0 was initiated at an open public workshop in July 2014). The group is also working with more than 75 organizations to develop methods to use these validated reference materials to understand the measurement performance of sequencing instruments and bioinformatics work flows.

The group is also developing standards for cancer diagnosis and therapeutics, such as candidate NIST SRM 2373, which consists of genomic DNA samples that have been extracted from five human breast cancer cell lines with HER2 gene copies ranging from no amplification to low, medium, and high levels. It is evaluating additional copy number standards for the cancer genes MET and EGFR and working on mixture designs for genome scale measurement assurance by establishing reference materials and methods for RNA-sequencing experiments using samples made from well-established mixtures of (usually three) human tissue total RNA isolates.

The group is also working on microbial detection and quantitation with qPCR. In partnership with their colleagues at the Institute for Bioscience and Biological Research (IBBR), they have developed yeast strains with nonnative sequence inserted into the yeast genome (sequence inserts are derived from SRM 2374) to use as controls for microbial detection methods that rely on detection of genomic DNA sequences. In principle, qPCR or other sequence-based assays can be validated by using the inserted sequence as the putative target. This work was initiated to support DHS validation needs. The group is developing four microbial strain whole-genome reference materials intended for use as reference samples to understand sequencing performance.

Opportunities and Challenges

Based on the publications, patents, and discussions, the BBD evinces scientific expertise on a par with that of leading researchers in the areas being researched and developed. However, the talent pool is stretched to capacity. It will be challenging for the BBD to set priorities and cut programs if necessary, because every research area for which the BBD is developing standards, measurement science, and validation of methodology is of great value to the biological and life science arenas.

The Bioassay Methods Group has developed potential intellectual property and could be a very valuable partner for NIH by providing controls and reference materials that NIH lacks for research studies. The group is demonstrating that biology is indeed greater than the sum of its parts. The newly formed engineering biology team has the potential to accelerate innovation and broadly impact the ability of U.S. companies to compete in the global marketplace for biomanufacturing and synthetic biology. The team is working on ways to enable quantitative measurements of complex biosystem behaviors and enhance the ability to extract predictive and actionable knowledge from data about complex biosystems. There is great potential in the stem cell area, which would benefit from predictive modeling. The group's challenge is to find ways to formally partner with NIH and the FDA as well as with industry to ensure continual resources, because the area of bioassays continually changes with the integration of improved technology and new information produced by the research community.

The Biomaterials Group is well positioned for expansion and taking a leadership position to coordinate all NIST biomaterial reference materials and standards. Its achievements are many, and it is in high demand from several health industries that are developing novel scaffolds for tissue engineering and protein-to-protein interactions. The research being done using BCARS microspectroscopy for digital pathology is impressive. The need for its capabilities is going to grow, and the challenge will be to keep up with all the stakeholders' demands. This group is also a very strong research partner for NIH, from which funds could be supporting some of the programs within this group.

The Cell Systems Science Group is involved in and performing many cutting-edge experiments and building integrated research programs that are leading to some very advanced technologies. The opportunities are almost endless in medical research and will multiply in the agricultural arena, in which the group is not currently much involved. Some businesses could be spun out of this group. One of their challenges is managing the amount of data they are collecting. The very broad scientific community that they work with is going to demand more from this highly trained and competent team of scientists.

The Genome Scale Measurement Group, partnered with Stanford University, has many opportunities for collaboration with small and large biotechnology companies in the San Francisco Bay area, which are diverse and numerous. This group has set up a beachhead for the MML on the West Coast and can serve as a conduit for many of NIST's programs. The research science is exciting and addressing large gaps and needs in the "-omics" sciences. The opportunity to hire postdoctoral researchers from Stanford and the other eminent research universities to work for NIST without their having to relocate to the East Coast provides an advantage with respect to bringing in new talent from the West Coast. Geographical distance between the two sites is a potential challenge. However, they communicate well through use of social media and other conferencing technologies. Another challenge is the cost of living in the Bay area. It would be worthwhile to consider salary adjustments for employees who are assigned to the Stanford campus.

Overall Assessment of Technical Programs

Research at the BBD is cutting edge and on target in addressing needs in biology and life sciences measurement technologies. The output of the BBD is measured by the output of publications and reports as well as by the reference materials and standards for measurements it has provided. The BBD is doing very well in the publication arena given that many of their papers are published in tier 1 scientific journals.

The quality of the research reviewed is very good, and each group is on target to reach the stated technical objectives. The Stanford model appears to be working and may be worth repeating in different parts of the country.

The BBD has demonstrated an impressive ability to leverage talent from other divisions and from other parts of NIST to grow its programs. However, the BBD is understaffed, considering its mission statement. One example is in the microbiology application arena: The research focus is very much on target with both the human biome and food safety and security research, and although the group is very small compared to some university departments, the quality of its work is outstanding and would be of interest to the U.S. Department of Agriculture (USDA) and the Department of Defense (DoD).

The BBD's scientific expertise supports NIST's technical programs at a very high level of quality and, in some cases, quantity. Working in the diverse areas of health care, manufacturing, food safety, environmental health, and national security, the BBD has a commendable grasp and knowledge of the gaps and needs as well as the ability to foster innovation and strategic partnerships. One concern is what can be done today to ensure not only stability of the groups but also strategic partnerships with other federal laboratories and research universities. The BBD stays very focused on its mission and has put into place people and programs to implement the goals of its mission.

PORTFOLIO OF SCIENTIFIC EXPERTISE

The Bioassay Methods Group is highly trained and motivated to bring quality assurance and quality control methodology to the novel tools being developed that will both qualify and quantify biological activity, wellness, predisease, and disease. This group has impressive researchers doing cutting-edge research; they effectively collaborate within and outside of the group to leverage needed talent.

The Biomaterials Group is focusing on areas that are very current in biotechnology. It possesses a highly qualified staff and a strong external network of collaborators at the federal agencies and in industry and academia. Demand for the services of this group is likely to grow in the next 2 years.

The Cell Systems Science Group has a major focus in medical research and is at the center of many of the major research programs being undertaken by NIH and pharmaceutical and biotechnology companies.

The expansion of the Genome Scale Measurement Group to the West Coast is good for the BBD. It establishes a footprint on the West Coast and will attract new talent to work on genomic science, which is in great need of reference materials, controls, measurement science, and validation. The highly creative and trained NIST group at Stanford is doing well and continues to try to include the Gaithersburg staff in many platforms and in developing and/or expanding their capabilities. This expanded center of excellence model is a good one; the MML might consider developing more of these types of partnerships.

ADEQUACY OF FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

The BBD laboratories visited are well equipped with the latest and best equipment for doing research in biotechnology. In addition, the scientists are very good at tweaking the instruments to do more and at integrating systems and creating new instruments. Given that biotechnology is a rapidly evolving technology and that the BBD is trying to anticipate emerging measurement needs as well as hiring and training experts to provide results that have an impact in biotechnology standards and measurements, overall the division has done an excellent job of acquiring the best tools in the toolbox to advance the understanding of complex biological systems on many fronts and at many levels.

The facilities visited were designed for maximum output and very well kept with respect to clean laboratory benches, well-stocked supplies, and a good flow of laboratory capabilities. The equipment of the BBD is state-of-the-art. There are several instruments that will support advances in the understanding of cancer therapies. As an example, within the Genome Scale Measurements Group's laboratory, near-state-of-the-art sequencing technology is deployed, with four different platforms (Illumina HiSeq 2500, Illumina MiSeq, Life Technologies SOLiD 5500W, and Ion Torrent PGM). There is also access to other sequencing platforms at the FDA, NIH, Mt. Sinai School of Medicine, and Stanford University. Another example is the protein preservation project, whose facilities include a novel, red-edge tabletop fluorescence instrument—a real advantage in understanding protein–protein interactions. The dental materials program has unique capabilities to simultaneously measure curing kinetics, stress evolution, and reaction exotherms of photopolymerized materials—another advantage in having companies work with the BBD.

Given that the tools in the biotechnology toolbox are continually being redesigned for more quantitative analysis, to remain competitive, purchasing new or retrofitting existing equipment will be high on the investigators' list. Partnering with instrumentation companies is something that the BBD already does extremely well; it is important that it continue to seek companies that have developed the next generation of biotechnology tools for alpha and beta testing and obtain the instruments at a reduced cost.

With respect to human resources, the BBD is a lean but highly productive division. It is effective and efficient regarding output, considering such a lean staff. The BBD manages to achieve its stated objectives even with its small staff, diverse thrust focus areas, and four major programs. The ratio of Ph.D.s to technicians is high, and in some applications more technicians could be employed to carry out some of the required maintenance of reference standards. The BBD management needs to consider adding more staff to the four divisions if it is going to continue to lead and form strategic partnerships for measurement standards, reference materials, and validation within the many and varied areas of biotechnology.

Working mainly in the biotechnology arena, the BBD has both challenges and opportunities. This unique group of scientists, whose expertise includes biology, chemistry, mathematics, computation, engineering, and physics, is addressing well the complex biological sciences that are continually in flux and driven both by policy and regulatory issues that seem to change frequently. Recognizing that there is a need for better measurements and standards for data sharing, reproducibility, scale-up, and commercialization, the BBD is working on the right things at the right time. For example, it is working in microbial measurements, cell manufacturing and therapies, synthetic biology, and predictive biology. However, there is not a critical mass in any of these areas sufficient to make the BBD a focal point for more outside collaborations.

The new programs in microbial measurements, cell manufacturing and therapies, and predictive biology hold great promise for huge successes. All three areas are being invested in today within the field of biotechnology. Without the required personnel and the right infrastructure, these three programs may not reach their full potential. These programs are also reaching out across the MML and to other laboratories at NIST to leverage resources and talent. The vision that stimulated the creation of these programs is commendable.

The BBD appears to have deep technical expertise in measurement of biological systems and is developing the same capacity for bioengineering. The caliber of the science being performed at the BBD is excellent. The staff are very motivated, highly trained in their respective fields, and enjoy working at NIST. The groups are working well together, and morale appeared to be high. They believe in BBD's mission and want to do as much as they can. They choose programs and projects in a strategic manner by integrating strong stakeholder input and aligning outside capabilities to their internal strengths. A good example is the collaborative program at Stanford University on advances in biological/medical measurement science, where they are in the heart of biotechnology entrepreneurialism and commercialization at Palo Alto, California. Access to faculty and students at Stanford is a win-win for both the BBD and Stanford. This model seems to be working with the other partners they have at the University of Maryland's IBBR, located in Rockville, Maryland.

The group leaders appear to communicate and work well together. They are respected and admired by the scientists and technicians at the BBD. Their knowledge of what is going on in many fields and their network of scientists outside of NIST is impressive. They know that they have to attend external meetings, deliver presentations, and publish as well as patent their findings. There is a can-do atmosphere, especially on the innovation and entrepreneurial—bench-to-bank—side of the equation to meet societal needs. A concern is the lack of effective communication with a broad customer base and stakeholders. The BBD needs to do a better job of marketing itself, including making its website easier to navigate.

With respect to human resources, there appears to be a need for the BBD to help the human resources professionals to develop improved ways to recruit the talent that the BBD needs. The challenge is to retain the early-career scientists by devising ways to recognize their many contributions and providing incentives to stay. New policies for promotion that include various tracks for promotion would be welcomed. Excellent hires of research staff at all levels have been made, with one recently hired scientist targeted to enhance the microbial program. The motivation to succeed appears to be infectious across the groups within the BBD.

DISSEMINATION OF PROGRAM OUTPUTS

The BBD is well driven by the stakeholder needs, and its continual outreach to federal agencies, academia, and industry is commendable. The publications were very impressive, especially those published in *Science, Nature,* and *Proceedings of the National Academy of Sciences*. The BBD needs help in filing more patents and licensing/codeveloping more of the creative innovations and technologies developed in its laboratories.

However, the BBD staff are not as effective or efficient as they want to be. They mentioned several lost or missed opportunities for commercialization. It appears that in order to better develop translational research outcomes, the BBD may have to perform a complete review and overhaul of their technology transfer operations. The BBD does not seem to be deriving optimal benefit from the NIST technology transfer mechanisms and the NIST Innovation and Industry Services (IIS) office. A good start to remedying the situation would be to review the BBD's accountability and outcomes for both the technology transfer office and IIS and see if other units are getting better input and support from these two offices, which are responsible for interfacing with industry and moving technology out the doors of NIST. Better integration and coordination between the BBD and the NIST public relations, communication, and IIS offices would enable the BBD to do more monitoring and more external customer interactions. The BBD is doing a relatively good job of monitoring stakeholder use and the impact of the program outputs. They have a very diverse group of stakeholders, as evidenced in Table 4-1.

The MML created the position of safety program coordinator, and it holds an annual safety day. It also developed an online system for hazard review and approval that is now used by other operating units, and it designed an iPad tool for safety inspections that was piloted in the MML but built for all of NIST to use. This could be an application that research laboratories would purchase. In addition, the newly created Office of Data and Informatics will enable much more data to be shared and examined throughout the MML and especially within the BBD.

There is a need for biological measurements and reference materials if the United States is to remain in a leadership position in both biotechnology and the life sciences. NIST's creation of the BBD by integrating some divisions has proven to be a very successful decision. The BBD's stakeholders and areas of applications are many, as illustrated in Table 4-1.

The number of the BBD's industry partnerships and its knowledge of which companies to contact and collaborate with are impressive. The number of partnerships with other federal laboratories and nonprofit institutions is equally impressive. The BBD is planning to do more external communications. The challenge, given the current budget and human resources, is how to keep all these major stakeholders involved and at the same time grow the programs to include more stakeholders. The opportunities are many and significant, considering the capabilities and instrumentation within the BBD. Additional staff and equipment will be needed to stay at the forefront of biotechnology, which is a moving target with many anticipated emerging measurement needs. The BBD needs to continue developing the expertise to make an impact in the field and at the same time create and increase more effective and efficient communication with their very broad base of customers and stakeholders.

TABLE 4-1 Major Stakeholders for the Measurement Technologies and Application Areas Within the BBD

Measurement Technologies	Application Areas	Major Stakeholders
Genomic metrology	Clinical diagnostics Cancer biomarkers Synthetic biology Microbial identification	FDA, NCI/EDRN, ABMS, DHS, FDA
Cell measurement assurance	Nano-EHS Cell-based therapies Synthetic biology Cell line ID	ISO, NNI, ARM, NIH/CRM, ISO, Liber Institute, ASTM, JCVI/ABMS, FDA, Academia, Biopharma
Imaging and spectroscopy technologies	Benchmarking/calibrations BCARS microscopy Live single cell analysis Flow cytometry	Pharma user facilities, ISAC, Academia, Cleveland Clinic, P41, MedImmune, ITL Big Data, ISAC, NIBSC
Biomaterials	Cell–materials interactions Materials characterization Protein stabilization	FDA, ASTM, NEI, ISO, ADA, NIDCR, Dentsply, 3M, Eli Lilly, MedImmune, Academia

NOTE: ABMS, American Board of Medical Specialties; ADA, American Dental Association; ARM, Alliance for Regenerative Medicine; CRM, Center for Regenerative Medicine; EDRN, Early Detection Research Network; ISAC, International Society for the Advancement of Cytometry; JCVI, J. Craig Venter Institute; NEI, National Eye Institute; NIBSC, National Institute for Biological Standards and Control; NIDCR, Institute of Dental and Craniofacial Research; and NNI, National Nanotechnology Initiative.

Metrology is based on three elements: traceability, measurement uncertainty, and method validation. The BBD is developing a very strong metrology base for biotechnology and the life sciences arena. The BBD is meeting many of biotechnology's current and future needs to enable U.S. competitiveness and global leadership. It needs to work more on informing others about its programs, and it needs to work on obtaining external resources from industry. The division is to be congratulated for achieving so much in such a short time. The leadership and staff work closely as a team; they are well-polished, well trained, and very focused.

FINDINGS AND RECOMMENDATIONS

The BBD has many cross-cutting activities within and outside of NIST. BBD staff work closely with the MML divisions engaged in the fields of manufacturing, biomanufacturing, biosciences, health and safety, security, and forensics. Overall, the division possesses a high level of technical skills and works on cutting-edge science that requires both reference materials and standards. They perform work in many areas with only 54 full-time equivalent staff. The division is lean in administration and technicians but has a good selection of Ph.D. scientists at all levels, from junior to very senior fellows. They have learned to leverage resources very well and chose strategic partners that can enhance or complement their in-house skill sets and capabilities. Unfunded mandates from Congress detract from programs from which funding is taken to address the unfunded mandates.

Recommendation: Where appropriate, the Biosystems and Biomaterials Division should address the potential resources from other agencies (e.g., National Institutes of Health, the Food and Drug Administration, the Department of Defense, and the Department of Justice) that would benefit from the Biosystems and Biomaterials Division's addressing these mandates.

BBD staff reported that the procurement procedure is a barrier to getting much-needed supplies on time; procurement dollar limits and procedures imposed by the Department of Commerce delay the ordering of supplies and the conduct of business with external entities; limitations on and administrative procedures for securing approval for attending meetings and for associate travel are counterproductive; and the human subject review, which is critical for success of many BBD projects, often gets bogged down.

Recommendation: The Biosystems and Biomaterials Division should work with those responsible for human subject review to accelerate human subjects review.

BBD staff reported that there is a disconnect between various central administrative functions and the BBD laboratories with respect to appreciating the needs of the scientists and how to make BBD capabilities known to potential stakeholders, clients, and the public. For example, BBD staff reported that there is little communication between the technology transfer group and laboratory staff. The BBD staff do not believe that they have had good interaction with and support from the technology transfer group at NIST and believe that the group responsible for innovation and industry services (IIS) has not adequately supported the scientists. They noted that the IIS met with them only once in the past few years. To make their work better known, the BBD might consider updating their NIST webpage to include videos, stories, and more pictures.

Recommendation: The Biosystems and Biomaterials Division should work through the Material Measurement Laboratory with NIST central operations to identify ways to achieve more effective and efficient service from those operations. The Biosystems and Biomaterials Division should also examine ways to improve and invest in more outreach and marketing of its many capabilities and should consider improvements to the web pages describing its activities.

There is no program in place to train junior scientists to take over the maintenance of the standards that are developed. Currently the Ph.D.s maintain the standards. Some Ph.D.s do not object to that, but others prefer to do more research. There is also a need for a succession or protégé plan; currently, succession planning is performed as needs arise. This has engendered concern that in the absence of a clear plan the younger researchers are restless and would probably leave if the economy improves.

Recommendation: The senior staff members should be given greater choice and/or more support with respect to responsibility for maintaining standards over several years. Promotion paths should include parallel tracks that consider basic, applied, and enablement science.

There are few bachelor and master's degree level technicians that could take on some of the more repetitive work currently being done by the senior staff. The BBD also needs to expand its working relationships with academic and industry partners.

Recommendation: The Biosystems and Biomaterials Division (BBD) should develop a program that involves interns from universities throughout the year to create more partnerships and potential workforce development for the BBD and/or establish a fellow program to bring in scientists from industry to work at the BBD and perhaps co-develop new products and processes as well as measurement technologies.

BBD staff noted that laboratory equipment purchases are overtaxed and that there has been a reduction in the amount of money for equipment purchases and maintenance contracts. Equipment has an institutional overhead cost of 30 percent to pay for human resources, safety, and other infrastructure support. BBD staff indicated that equipment taxes significantly reduce the amount of equipment they can purchase.

Recommendation: The Biosystems and Biomaterials Division should examine alternative paths to acquire equipment, including cost sharing with and borrowing from other agencies, where feasible.

The BBD depends on the materials with which they work, but they do not have the capability to make the materials.

Recommendation: The Biosystems and Biomaterials Division should plan for material purchases when preparing budgets and should consider negotiating with industry to have them made and then validated by the Biosystems and Biomaterials Division.

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Chemical Sciences Division

The Chemical Sciences Division (CSD) consists of 170 staff members located in Gaithersburg, Maryland (the primary site) and at the Hollings Marine Laboratory in Charleston, South Carolina. This division was formed during the recent laboratory reorganization by combining approximately two-thirds of the staff from the former Chemical and Biochemical Reference Data Division and the Analytical Chemistry Division. The CSD integrates mainstream chemical sciences expertise into one organization in order to provide strong fundamental research and measurement services across several key technical programs. The CSD defined its mission as follows:

> The Chemical Sciences Division provides the measurement science, standards, instrumentation, technology, data, and chemical informatics required to support the nation's needs in the determining chemical composition, quantitation, and chemical structure and in the measuring of a wide variety of chemical properties and processes, such as chemical reactivity and mechanisms as well as thermochemical properties. In partnership with U.S. industry, other government agencies, and other scientific institutions, the division performs fundamental and applied research to advance and create state-of-the-art measurement capabilities, theory, and computational methods for quantitative measurements and sensing of solids, liquids, gases, plasmas, transient species, and multicomponent matrices. The division also formulates and disseminates reference materials, measures, and critically evaluated reference data. These activities support the chemical science, technology, and engineering enterprise with the intent of fostering innovation and confidence in measurements and technologies used in a wide range of applications, including chemical analysis and separation, environment, health care, sensing, manufacturing, and energy transformation.[1]

ASSESSMENT OF TECHNICAL PROGRAMS

Accomplishments

The CSD has five main technical thrusts in which several leading capabilities and technology areas have been established: environmental sciences, climate science, biomedical and health, nutrition, and materials measurements. Several advances have been made in all of these thrusts in the last 2 years. The thrusts track well with the cross-cutting programs in the Material Measurement Laboratory (MML). Of the MML cross-cutting programs, the CSD contributes the greatest number of staff for the environment, climate, and food and nutrition programs, is a major contributor to three programs (biosciences and health, energy, and manufacturing), is a minor contributor to five programs (advanced materials, NanoEHS initiative, materials genome initiative, additive manufacturing initiative and safety, security, and forensics), and does not contribute to the biomanufacturing initiative or physical infrastructure programs.

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[1] NIST Material Measurement Laboratory, "2014 National Research Council Assessment of the NIST Material Measurement Laboratory-Read-Ahead Materials," Gaithersburg, Md., June 2014.

Environmental Sciences Thrust

The environmental specimen bank, located at the Hollings Marine Laboratory, is a unique national facility that ensures the archiving of marine specimens and materials to enable scientific studies of the environment and is the focus of considerable development of standard reference materials (SRMs) and measurement methods. This cryogenic banking facility contains a wide range of marine specimens of interest to many regulatory environmental and resource management agencies, the wildlife health community, university researchers, private organizations, and international environmental organizations. More than 85,000 aliquots of approximately 20,000 specimens are archived in this bank dating back to the 1970s. A more efficient bar-coding system has been developed that allows for reduced time in processing and retrieving samples, and a new banking and analytical program has been established for assessment of threats to coral systems. Much work has gone into measuring contaminants that are not yet regulated but are of toxicological concern. Researchers are developing nontargeted screening methods in this area, which has taken advantage of their strengths in chromatography and mass spectrometry, along with computational tools for enhanced data analysis. This group has studied several families of persistent organic pollutants (POPs) and has developed and distributed 140 SRMs for this important area. They have also applied these instruments and data analyses to analyzing the antioxidative properties of dietary supplements.

Another area within this thrust involves the environmental health and safety aspects of nanomaterials. This group is actively seeking to develop measurement tools, methods, protocols, SRMs, reference materials, and validated data and models to enable other organizations to measure properties of nanomaterials in relevant media. It has successfully utilized a new system, coupling electrospray-differential mobility analysis (ES-DMA) with inductively coupled plasma mass spectrometry (ICP-MS), and has made advances to the existing single-particle inductively coupled analysis plasma-mass spectrometer (spICP-MS) to measure elemental compositions of nanoparticles as a function of size, nanoparticle density, and ligand packing density on the their surfaces. The spICP-MS analysis can be performed with existing ICP-MS systems, making this method potentially useful for real-world applications in other laboratories. An ISO standard document is being prepared on this technique, and the group has produced several SRMs related to nanomaterials.

Climate Science Thrust

This thrust entails multiple activities related to the advancement of chemical metrology and data analysis tools for environmental research, assessment of climate change, and related policy development. The group continues to develop critical capabilities related to chemical processes. Many studies have been carried out in order to determine key areas of interest such as determination of reaction mechanisms, measurement of rate constants, transport properties, and the transformation of chemical species in both gas and liquid phases. These studies have provided critical reference data and standards that are widely disseminated throughout the United States and internationally. Another key area of expertise is in gas sensing metrology. This group has provided critical certified reference materials for many of the major greenhouse gases, as well as other important areas of gas metrology such as those related to energy, air quality, and emissions; the group has been serving as one of the central calibration laboratories for the Global Atmosphere Watch Program of the World Meteorological Organization. The group maintains a wide portfolio of gas mixture SRMs and has developed and implements an efficient dissemination process through its NIST Traceable Reference Material (NTRM) program. The quality of the SRMs in this area is well documented in international comparison programs, with the performance of NIST SRMs equaling or leading the top four laboratories in the world in terms of accuracy and low uncertainty. The recent inclusion of highly accurate spectroscopy expertise and activities into this group has enabled much closer linking of the NIST SRM and standard reference database (SRD) products in this area. The group's utilization of cavity ring-down spectrophotometers allows measurement accuracy that is the current state of the art, is recognized worldwide (for example, by reviewers of journal articles), and is contributing to global spectral databases, such as the high resolution transmission (HITRAN) database, that are used for remote spectroscopic monitoring of atmospheric species and greenhouse gases These researchers have recently developed a patented method for high-speed, ultra-high-sensitivity laser measurements of gases, called frequency-agile rapid-scanning spectroscopy (FARS). This method provides an extremely accurate, high-bandwidth method for defining laser frequency detuning, and it can likely be adopted by instrument manufacturers for further dissemination.

Another area that has shown great progress within this thrust is the development of metrology and standard materials for aerosol monitoring. This group, in collaboration with the National Research Council Canada and the University of Maryland, has developed the ability to quantitatively measure mass traceable aerosol absorption and scattering cross sections. There are two permanent staff members and one postdoctoral researcher working in this area; they have several publications and are anticipating the ability to provide candidate SRMs for trial with research groups shortly. This progress has been achieved rapidly. The next stage could actively seek greater integration of these activities into other national and international programs that are assessing and monitoring the effect of aerosols on radiative forcing models for climate change. Another active area within this thrust is pH measurements. This group is carrying out careful research to provide a unified definition of pH in seawater that is consistent with the standard definition of pH in solutions with lower ionic strength, and it has produced multiple pH buffers in artificial seawater that can be used as calibrants for field measurements in these solutions. They have also utilized quantitative nuclear magnetic resonance (qNMR) to characterize the indicator dyes that are utilized in seawater pH measurements in climate change studies, and they have verified the purity of these dye batches for use in these studies.

Biomedical and Health Thrust

The division is well integrated into the larger biomedical and health programs within the MML. It provides critical support in the biomedical and health area by creating, supporting, and advancing the measurement infrastructure through new reference methods, materials, and data for clinically relevant chemical species in biologically relevant fluids. The group working in this area develops and maintains more than 50 reference materials for clinical diagnostic markers for routine assays in clinical and pathology laboratories. This group has also developed and maintains a series of SRMs for harmful common-exposure environmental, commercially or industrially relevant agents for use in workplace safety and health-focused regulatory agencies. This group in the metabolomics area develops and validates a wide range of technologies, including two-dimensional gas chromatography with time-of-flight mass spectrometry (TOFMS), liquid chromatography-mass spectrometry (LC-MS), and high-resolution NMR spectroscopy for the accurate determination of metabolites in biologically relevant matrices. Several clinically relevant SRMs have been released since 2012, and a series of reference materials are being developed in collaboration with the Centers for Disease Control and Prevention for a range of organic contaminants in human fluids. Researchers have developed and implemented three quality-assurance programs to assess the accuracy and precision of nutritional biomarkers of clinical relevance in serum and plasma materials, including fat-soluble vitamins and carotenoids, vitamin C, vitamin D metabolites, and fatty acids. These programs have been utilized in hospitals, clinical testing laboratories, medical research institutes, academic universities, and government research laboratories. Researchers have also been developing a metabolomic-based data hub, where specific quality control material of metabolomics-relevant data will be available on the Internet to ensure that the metabolomics community will have an indicator of quality for its work. This ongoing effort will need to be established and maintained with appropriate data analytics. This group has also developed a shotgun-based lipidomics mass spectrometry approach to detecting and semiquantifying hundreds of individual lipid species for faster profiling of lipid extracts from biological samples. These techniques have been applied in several biomedical and human health investigations.

Nutrition Thrust

The CSD has a large effort in providing standards, quality assurance, and measurements for the nation's need to identify and quantify chemical and biological species for the nutritional assessment of foods for use in labeling and for developing measurement methods to ensure that nutritional guidelines are met in the population. The group working in this area has been involved in measurements and SRMs for nutritional assessment of foods for more than 30 years, and more recently for dietary supplements and human nutritional status. It develops and maintains more than 50 reference materials and more recently has developed more than 25 food-matrix SRMs for nutrient content. This group has shown excellent technical leadership in the Vitamin D initiative with the National Institutes of Health Office of Dietary Supplements and has provided advanced isotope-dilution LC-MS for determining vitamin D metabolites in human serum, which have been utilized in international programs. A good example of a critical food-related SRM is the improvement of the original infant formula SRM (SRM 1846). This SRM included only four water-soluble vitamins in 2009 but has now been expanded, with certified values assigned for 43 nutrients using advanced analytical techniques and expertise in the group. A replacement standard was issued in 2011 with 46 certified and 46 reference values, which currently has sales of more than 520 units/year.

Another area of active research is the development of analytical methods for dietary supplements. This group is actively developing SRMs for several dietary supplements. Since 2002, a total of 38 botanical and nonbotanical dietary supplement SRMs have been issued. These are complex materials and have required that chromatographic separations and extraction procedures be specified for each of these materials. Several new analytical methods were developed, and regular monitoring is required for all of these materials, because their stability is unknown. Recently, species DNA identification was added as a certified property for *Ginkgo biloba* in SRM 3246, and the group is planning to incorporate this type of information into several other SRMs. This group has also maintained the quality assurance for the Dietary Supplement Laboratory Quality Assurance Program (DSQAP). The program was started in 2007 to provide a mechanism for the assurance of quality across many laboratories and to allow the laboratories to compare results with NIST and with the group consensus. More than 140 different laboratories have participated in these studies, and the comparative results are compiled and made available on the DSQAP website.

Materials Measurements Thrust

The CSD maintains and develops a large amount of advanced instrumentation in order to advance the measurement sciences in materials and to ensure traceability throughout different industries. This group produces and maintains more than 400 manufacturing-related reference materials, many of which are in the production and processing of metals, ores, and cements. Within the past 3 years, the group has been involved in producing and certifying approximately 30 new manufacturing-related reference materials. They have also carried out innovative approaches for industrially relevant processes. One example is a highly sensitive optical mass flowmeter that was developed for effective monitoring of atomic layer deposition (ALD) processes and then built at an industrial collaborator's facility for use in prototyping. The group has also developed reference spectra for this process. It has also developed a time-resolved surface-sensitive spectroscopic technique that allows careful study of surface reactions and precursor delivery during an ALD procedure on industrially relevant time scales.

Opportunities and Challenges

The combination of the strong spectroscopy expertise in the Measurement Science Group with the expertise of the Gas Metrology Group in the program has set the CSD as a leader in the field of climate science, and the division has a rapidly developing program on aerosol metrology. Combining the reference materials program with the reference data expertise has led to a series of reference materials and reference data products that are finding a lot of utility in various fields, and expansion of these activities is warranted.

The SRM program is very large and diverse. It is critically important for many industries and other national stakeholders, who are strong drivers of its expansion. The CSD research program is well integrated into this program and has excellent measurement science expertise and instrumentation to develop the new SRMs that are required to advance several fields important to stakeholders. However, balancing maintenance of the current portfolio of SRMs and development of the critical new SRMs that are needed in industry is a challenge that needs to be addressed.

The CSD needs to develop a strategy for maintaining and developing new SRMs and for optimizing the resources and staffing of SRM programs. Because the division maintains multiple SRMs that support specific sectors—diagnostics and food supplements—appointing a scientist with clearly identified responsibility for this group and for interaction with relevant stakeholders would bring benefits to both the CSD and stakeholders, and it would allow the CSD to develop strategies and scientific programs that address generic issues such as commutability of reference materials. A committee has been formed to develop a strategy for SRMs. The team needs to continue development of the strategy and to ensure that the proper stakeholders in industry are consulted as needed to develop a broad strategy for this critical national capability. CSD management needs to ensure that there is proper recognition for staff working in this area and that they maintain this emphasis. Developing SRMs and maintaining them can be considered different activities, and it may be effective to assign different staff to these two roles.

Overall Assessment of Technical Programs

The technical programs that are being addressed by the key thrust areas in the CSD are directly integrated into the mission of the MML and are in support of the key role that NIST serves for the nation. There has been significant progress in all of the key thrusts since 2012. This division maintains and develops the majority of the SRMs (approximately 1,000) at NIST, and it is continuing to broaden this portfolio to meet the needs in many key areas related to environmental, climate, biomedical, nutrition, and industrially relevant processes. Broadening into these new, more difficult SRMs is a key role for this group, whose expertise in measurement science across many different techniques is excellent. At the same time, it is necessary to maintain the other SRMs that are in the portfolio.

PORTFOLIO OF SCIENTIFIC EXPERTISE

The CSD has deep expertise across many different measurement science fields and has done a good job of attracting and retaining good talent. The majority of staff that were interviewed were highly motivated, excited by their work, and appreciative of the fact that they are working on important things for the nation. They expressed an appreciation of the freedom allowed in the pursuit of their work and the exploration of new ideas in line with the key mission of the CSD. In many cases, this division has done a good job of hiring new talent to maintain the succession of key technology expertise. The division has addressed this through new staff hires and postdoctoral researchers in a few areas, such as pH measurement, electrochemistry, and gas metrology. The CSD has also put highly capable people in new areas to expand their ability to address key challenges, such as in aerosol research for climate science. The recent reorganization of the division has enabled some researchers to work across areas that were not previously addressed; this will strengthen their scientific expertise through innovative collaboration. Several of the researchers noted that the collaborative nature of work at NIST drives such interactions regardless of organizational structures. The technical training program for new hires seems to be effective, and the new scientists have many interactions with the more seasoned scientists, which will ensure that this scientific portfolio remains strong and continues into the future.

While the CSD has done a good job on its succession planning in some areas, such planning needs to be extended to critical technology areas that do not have significant depth of expertise. One example of this is the inorganic mass spectrometry area, including isotope ratio work. This is an area where the MML's capability and expertise is recognized worldwide and the CSD is integrated into large international projects. This group does not have a clear succession plan, and there is a lack of staff members and postdoctoral researchers who could be groomed to work in this area. If the CSD hopes to maintain its world leadership in this area, it will need to consider succession planning more actively. Similarly, it needs to systematically evaluate all of its key technology areas to ensure that it has an active pipeline of early-career scientists being mentored by its seasoned experts. Succession planning also needs to be expanded to include a staged plan to develop the technical leadership necessary to assume group leader roles by giving prospects training and other leadership experience. It already utilizes project coordinator roles to provide such leadership training and needs to continue and expand such practices. Strategic collaborations to tap into scientific expertise outside NIST also need to be considered. Some programs have involved collaborations with other institutions, while others could potentially benefit from further collaborations.

The division needs to examine whether its programs have state-of-the-art facilities and expertise and to start collaborative research programs in areas that would help to accelerate its projects more effectively, such as aerosols, isotope ratios, and electrochemical analysis. Consideration also needs to be given to optimizing the ratio of Ph.D. staff members to technicians, particularly in the area of SRM maintenance (for example, renewal and stability studies). This work is done predominantly by Ph.D.s, but much of it could be transferred to well-trained technicians or outsourced, freeing the Ph.D.s for the more challenging work of developing new SRMs. This division has an SRM advisory group in place to optimize the overall SRM portfolio—that is, to decide which SRMs to phase out, which to maintain or replenish, and which new ones to develop— but the staffing model needs to be incorporated into this strategy as well. The CSD is the largest division in the MML and is successfully delivering SRMs and SRD, but no scientist within the division has been appointed a NIST fellow. As a motivator for staff, particularly early-career scientists, CSD management needs to work with MML management to continue to explore ways to provide recognition for science leaders in the division.

In summary, the CSD has very broad scientific expertise across multiple areas, including world-recognized expertise in gas metrology, spectroscopy, mass spectrometry, neutron activation analysis, and inorganic measurement science, and other areas, and the division is utilizing this expertise to solve major problems facing the nation. It is advancing several fields of measurement science in a targeted fashion, and it has good depth in succession planning across the majority of these fields. However, this succession planning needs to be expanded across all of the key technology areas to ensure that this scientific expertise can be maintained in the future.

ADEQUACY OF FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

The CSD has a large amount of state-of-the-art equipment and has continued to advance many of the measurement thrust areas at the forefront of technology. It has achieved several advances in mass spectrometry, including coupling electrospray-differential mobility analysis (ES-DMA) with inductively coupled plasma mass spectrometry (ICP-MS) and single-particle, inductively coupled analysis plasma mass spectrometry (spICP-MS). The division staff are respected worldwide for their capabilities in isotope ratio work, and the division is one of few facilities that are advancing the area of metal speciation with ICP-MS. The facilities housing cavity ring-down spectrophotometers and mass spectrometers are optimized to allow unprecedented measurement accuracy, and the researchers are advancing various fields of spectroscopy, including the patented high-speed ultrahigh-sensitivity laser measurements of gases, called frequency-agile, rapid scanning spectroscopy (FARS). In general, its facilities for gas metrology are highly advanced and allow them to study more greenhouse gases than any other facility of this type. The division's NMR facility in Charleston, South Carolina, is extremely powerful and broad; it contains an 800 MHz unshielded NMR and a 700 MHz shielded NMR, along with other spectrometers that can be utilized by researchers. These instruments are cryoprobes with triple resonance probes, along with a flow probe and a broadband probe, which allows for highly advanced testing of biological molecules and many other systems. The facility is optimized and built specifically for housing these instruments. The environmental specimen bank is a very important facility that has had significant upgrades, which include more efficient barcoding and specimen-banking expansion of the number of specimens. The NMR facilities in Gaithersburg are utilized by all MML divisions, and access to the instruments is being managed appropriately. The neutron activation facility is critical for analyzing ultratrace materials and for developing SRMs for a broad range of materials; it is among the most powerful in the world. The combination of instrumental neutron activation analysis (INAA), radiochemical neutron activation analysis (RNAA), prompt gamma neutron activation analysis (PGNAA), and delayed neutron activation analysis (DNAA) is extremely powerful by comparison with other elemental analysis laboratories in the nation.

Many staff members complained that space is limited for expansion or for new instrumentation to be purchased, as well as for visiting researchers or other increases in staff. Older or less utilized equipment is still present, contributing to the space limitations. The laboratory facilities are not organized to maximize the efficiency of work flow; for example, a sample may be weighed out in one laboratory, carried to another laboratory for analysis, and carried to yet another laboratory for further analysis. The CSD needs to perform an assessment of optimization of its laboratories, considering efficiency and instrument utilization, and considering the removal of outdated or underutilized equipment to free up valuable laboratory space.

Many instruments have been built, modified, or optimized. In some cases, computer programs have been developed by division staff. It is important for the division to continue to carry out these advancements in technology, but there is a risk to the maintenance and longevity of the equipment. For this equipment to remain usable 10 years from now, it needs to be able to interface with next-generation computers and other equipment. Because some of the equipment developed in-house is not supported by any instrument vendors, maintenance and repairs require NIST resources. Many of these instruments are maintained and used predominantly by a single user, limiting their utilization rates. These instruments are also used predominantly for one project area; they might be applicable to problems across other divisions. Instrument vendors might offer opportunities to manufacture the equipment, achieving greater longevity and more dissemination. Some instruments, like the two-dimensional online liquid chromatography-mass spectrometer (2-D-LC-MS), are now commercially available.

A matter of concern noted by the staff is that the overall procurement and contract process by which the division operates is impeding the implementation of technical programs and overall productivity by imposing excessive delays ranging from small consumable items to large capital purchases. Acknowledging that the CSD needs to operate under government procurement rules, its management needs to work with MML management and NIST administrative offices to provide greater connectivity, a common vision, and best practices for efficiency in this area. The CSD also needs to continue work with NIST information technology offices to achieve and maintain reliable information technology services, necessary for successful SRD dissemination.

In summary, the CSD has a very diverse and highly sophisticated instrument base and is driving the state of the art in many of the instrumentation areas. The facilities are in many cases carefully designed for the instruments that are located within them, but in some cases outdated equipment continues to be in use side by side with newer equipment. This space can be optimized for better productivity.

DISSEMINATION OF OUTPUTS

Since 2012, the CSD has produced 440 publications and 62 NIST internal reports. The division staff have also produced a series of guidelines leading to the standardization of new protocols for many technologies, including ISO TC229-Nanotechnologies, for the use of ICP-MS for analysis of nanomaterials, and a standard protocol for spICP-MS. They have co-authorship in a World Meteorological Organization (WMO) report, a report on the stratosphere-troposphere processes and their role in climate (SPARC), and of the WMO global atmosphere watch (WMO-GAW) guidelines for continuous measurements of ozone in the troposphere. CSD researchers have also provided documentary standards leading to the standard specification for handheld point chemical vapor detectors (HPCVDs) for homeland security applications (ASTM standard E2883-13). CSD researchers serve on more than 20 national and international standards development organizations and participate in industry roadmapping and consortia activities. Since 2012 they have also been inventors on more than 5 patents.

The CSD has produced more than 1,000 SRMs (more than 75 percent of the NIST total). In addition, CSD researchers disseminate critically evaluated data through a series of publically accessible databases, including the NIST Chemistry WebBook, accessed by over 13,000 unique users per day. The WebBook provides a wide variety of data on more than 80,000 chemical species, including three-dimensional geometrical structures; thermochemical data; infrared, ultraviolet, and visible spectrophotometry; mass spectra; ion energetics data; fluid properties; thermophysical data; and gas chromatographic and solubility data.

Although the standards program at the CSD is extremely wide-reaching, increased utilization of the program is dependent on effective and efficient contact with government and industry stakeholders. The establishment of a project coordinator position in food, nutrition, and dietary supplements has resulted in successful communication and interactions with key stakeholders and provided a clear entry point into NIST for these stakeholders. Leveraging this position more broadly in other sectors would provide clear technical representation of a sector and clear communication, outreach, and expansion of SRM utilization. The coordinator provides individuals with a broad overview and knowledge of NIST's services for a sector and is empowered to represent NIST. The CSD needs to provide recognition and rewards for such coordinators. It is also important that the CSD, in collaboration with industrial partners, define and collect data on metrics that identify the value that the division provides to industry. Understanding how industry utilizes the work from the CSD, including the collaborative work and the SRMs or other data offerings, would help the division to ensure that it is meeting the most important needs to help accelerate industrial success.

As a whole, the CSD is widely disseminating its work products through publication, reports, and guidelines for standardization; and by coauthoring climate reports; providing data on chemical species that are critically needed by industry, academic institutions, and other government agencies; taking part in standards development organizations; and selling a large number of SRMs. This wide variety of work is utilized by many organizations to improve scientific measurements and help to shape national policies pertaining to climate, environment, health, energy, and nutrition, using the most accurate data obtainable.

OVERALL ASSESSMENT

The CSD is meeting its mission and functional goals and is providing many key measurements, data, and standards that are critical for the nation. The technical thrusts are aligned both with many of the key technical programs at NIST and with key problems facing the nation. The scientific expertise is broad across multiple areas, and the CSD is actively working on succession plans to maintain key expertise areas. The equipment and facilities are in many cases state-of-the-art, although there are issues with space management and the required capital to maintain this equipment base. There are many efforts to disseminate the work broadly, including a good publication record, a few patents, and a large number of critical SRMs and other data products (like the NIST Chemistry WebBook) that are utilized by huge numbers of people in industry, academia, and other agencies.

The reorganization of the division has yielded some of the desired synergies, such as the strong spectroscopy and spectrometry expertise, enabling key measurements with greater accuracy to support the development of standards for climate science, and enabling integration of reference materials and reference data expertise to generate a series of reference products across several important areas. The division has put in place a strategy for motivating, supporting, and evaluating staff publication in high-impact and other peer-reviewed journals. However, the publication rate has remained fairly constant since 2009, and the clear divide between the researchers who are working on SRMs without publication potential versus other research that can result in publication, is a challenge that the division is continuing to address. Since 2009 the CSD has added staff in gas metrology, electrochemistry, and NMR spectroscopy and has made significant strides toward developing an atmospheric aerosol program. The reliability of the information technology infrastructure has been improved to 100 percent to avoid interrupted access to the databases. Although improvements have been made, there are still issues with unplanned network shutdowns.

FINDINGS AND RECOMMENDATIONS

The CSD has a very large SRM program, critically important to industry and government stakeholders. Their research program is well integrated into the program to develop new SRMs that are required to advance several fields. Balancing the maintenance of the current portfolio of SRMs with developing new SRMs that are needed in industry is an identified challenge that needs to be addressed.

Recommendation: The Chemical Sciences Division should continue to develop a strategy for maintaining and developing new standard reference materials and standard reference data and for optimizing the resources and staffing that support programs, including the balance between Ph.D. scientists and technicians.

Recommendation: The Chemical Sciences Division should ensure that the proper stakeholders in industry are consulted to develop a broad strategy for its development of standard reference materials and standard reference data.

The CSD has addressed the issue of succession planning in technical areas by hiring new staff and postdoctoral researchers in a few areas, such as electrochemistry and gas metrology. The technical training program for new hires seems to be effective.

Recommendation: The Chemical Sciences Division should formalize its succession planning and expand it to areas with low staffing levels. The Chemical Sciences Division should include in its succession planning a strategy to develop the skills and competencies needed to be effective group leaders and should consider the project coordinator role an exemplar.

Recommendation: Chemical Sciences Division management should ensure that there is proper recognition for staff working on development of standard reference materials and standard reference data.

Staff in some programs collaborate extensively with other institutions, while those in other programs could benefit from such collaborations.

Recommendation: The Chemical Sciences Division should examine its programs to identify which facilities, equipment, and expertise are state-of-the-art and should initiate

collaborative research programs in areas where collaboration would accelerate projects, such as aerosols, isotope ratios, and electrochemical analysis.

Space is limited for expansion and for new instrumentation. However, the space is not optimized; older and less-utilized equipment is still in place and contributing to the shortage of space. Additionally, the laboratories are not organized to optimize the efficiency of work flow.

Recommendation: The Chemical Sciences Division should identify ways to optimize work flow in its laboratories and should consider removing outdated or underutilized equipment.

CSD staff noted that the procurement and contract processes at NIST impede the implementation and productivity of technical programs by causing excessive delays ranging from small consumable items to large capital purchases.

Recommendation: The Chemical Sciences Division should work with Material Measurement Laboratory management and NIST administrative offices to provide greater connectivity, a common vision, and guidance on best practices to make procurement more efficient.

Provision of several standard reference data sets is dependent on having reliable NIST information technology services. CSD staff reported that the reliability of these services at the CSD is suboptimal.

Recommendation: The Chemical Sciences Division should continue to work with NIST information technology offices to achieve and maintain reliable information technology services, which are necessary for successful Standard Reference Database dissemination.

Utilization of the outputs of the CSD standards program depends on effective and efficient contact with government and industry stakeholders. The establishment of a project coordinator role in the areas of food and nutrition and dietary supplements has resulted in successful communication and interactions with key stakeholders and has provided a clear entry point into NIST for these stakeholders. This role provides these individuals with a broad overview and knowledge of NIST's services for a sector and empowers them to represent NIST to the external community.

Recommendation: The Chemical Sciences Division should expand application of the project coordinator role to additional Chemical Sciences Division thrust areas and should explore ways to provide recognition and rewards to project coordinators.

6

Materials Measurement Science Division

The Materials Measurement Science Division (MMSD) was created by the merger of the former Ceramics Division of the Materials Science and Engineering Laboratory, the Surface and Microanalysis Science Division of the former Chemical Science and Technology Laboratory, and the Securities Technology Group, formerly part of the Office of Law Enforcement Standards. This is a large division, with more than 160 employees spread over eight buildings.

The MMSD provides the measurement science, measurement standards, and measurement technology required to enable characterization of materials in support of the nation's needs. The work emphasizes the determination of the composition, structure, and properties of materials. The technical work is divided into eight groups: Microscopy and Microanalysis Research Group, Nano Materials Research Group, Materials for Energy and Sustainable Development Group, Surface and Trace Chemical Analysis Group, Synchrotron Science Group, Materials Structure and Data Group, Nanomechanical Properties Group, and Security Technologies Group.

The eight groups share a common umbrella of characterization of the structure, properties, and composition of materials. The research topics range broadly from fibers used in soft body armor systems, to crystal structure determination of materials, to surfaces and nanoscale systems. The research topics are roughly organized by four main technical thrust areas: advanced manufacturing; advanced materials; safety, security, and forensics; and sustainability and energy. However, at this early stage of the MMSD the scientists seem more closely aligned with their particular group rather than with the research thrust areas.

ASSESSMENT OF TECHNICAL PROGRAMS

Accomplishments

The Microscopy and Microanalysis Research Group performs research in, and development of, microscopy and microbeam analysis techniques for the compositional, morphological, and crystallographic characterization of matter down to atomic spatial scales. The instruments use excitation by beams of electrons, ions, and photons. The group develops improved methods of quantification as well as documentary standards, SRMs, and SRD. These techniques are used effectively to address problems in materials science and chemical science, semiconductors, optoelectronics, environmental and biological sciences, and processes.

The Nano Materials Research Group develops standards and innovative metrology to advance nanomaterial research and applications for the benefit of U.S. commerce. Its goals are to determine the physical and chemical properties of a wide variety of nanoscale organic, inorganic, biomolecular, and hybrid systems, resulting in standards, methods, reference materials, and measurement data to advance a wide range of technologies and stimulate innovation.

This technical thrust is focused on advanced materials on the nanometer scale, addressing topics such as developing actinide microspheres for validating spectroscopes, adsorption of monolayers, cross-cutting work on the structure and properties of nanowires, advanced manufacturing, and device fabrication. All these topics are in response to the needs of industry and other federal agencies.

The Materials for Energy and Sustainable Development Group has performed work on a portfolio of fabrication and characterization techniques, with emphasis on energy harvesting, energy efficiency, and CO_2 capture. Two closely related projects involve the deposition of phase-spread heterogeneous thin films. This thin film technique is applied to Seebeck coefficient certifiable standards and the high-throughput combinatorial screening of multicomponent systems. This supports sustainable development because it holds promise for converting industrial waste heat to electrical energy. The same high-throughput screening technology was applied to passive smart window coatings that exhibit temperature-dependent infrared reflectivity. A closely related metrology advance is the development of an nJ-sensitivity nanocalorimeter, which can be used to study phase changes in thin films. This group also collaborates with the Department of Energy's (DOE's) National Energy Technology Laboratory in the characterization of metal organic framework structures that have been proposed for use as CO_2 scrubbers. These projects are very relevant and timely, and they exploit the unique analytical and metrological resources of the MMSD. The combinatorial high-throughput studies are also highly relevant to the Materials Genome Initiative. This group is making efficient use of high-quality instrumentation to address selected problems ranging from specific research on high Seebeck thermoelectrics to globally significant carbon capture and mitigations. This field is highly competitive and fast moving. Care is needed in selecting problems where MMSD strengths can be leveraged.

The Surface and Trace Chemical Analysis Group conducts research on the chemical and structural properties of matter by applying various ion- and photon-based microscopies to provide spatially resolved elemental, isotopic, and molecular information. The group studies the fundamental aspects of the excitation process and addresses quantification, standards development, instrument improvements, and data analysis challenges associated with these analytical methods; the group applies the methods to autoradiography and nuclear track methods, size calibration of particles, trace detection of explosive and narcotic particles, and advanced flow visualization.

The Synchrotron Science Group develops and disseminates science and technology pertaining to the measurement of structure, including chemical and electronic, of advanced materials by synchrotron methods. This is a long-standing and extremely productive collaboration between NIST and DOE. The primary focus is on spectroscopy and microspectroscopy techniques that span the soft to hard x-ray regimes. There is a significant investment from NIST to build, maintain, and support the synchrotron measurement capabilities at the National Synchrotron Light Source (NSLS) I/II; it also places staff and associates at the Brookhaven National Laboratory.

The Materials Structure and Data Group is concerned with the measurement of atomic structure using neutron and x-ray techniques and with electron microscopy. There is a complementary first-principles modeling effort. The group is also concerned with the essential, challenging job of developing uniform electronic means for communicating and navigating such complex data sets as phase diagrams and crystallographic structure determinations, which formerly were archived graphically in journals and books, and which use a variety of different arcane naming conventions. Current structure and imaging work is complementary to other MMSD efforts, including the imaging of thin films for photovoltaics. The curation and dissemination of structure and phase data are essential to the Materials Genome Initiative and to compliance with the Digital Accountability and Transparency Act (DATA). The materials and structure database has also yielded fruit by permitting automatic checking of historical data for internal consistency. This group maintains SRD on crystallography and structure (SRD 3, 83, 84) and phase equilibrium (SRD 31) and provides associated SRMs.

The Nanomechanical Properties Group develops measurement techniques for the mechanical response of submillimeter material. Recent successes include high-quality and high-throughput stress-strain relations on Θ-shaped machined samples (where samples are typically hundreds of μm for ceramics and 50 μm for metals) and the development and calibration of atomic force microscopy (AFM) flexural and torsional cantilevers, including cantilever SRMs. The stress-strain relations are approaching the ability to measure the response of individual grains. Another noteworthy achievement is the measurement of curvature of thin films using a specially modified x-ray lattice comparator. This work is unique and of the highest caliber. With NIST's historical contribution to fracture and failure, this work is poised to give the Materials Genome Initiative a solid database of reliable mechanical response that is particularly well-suited to understanding and validating multiscale models. The group is further developing a collocated nanomechanics clean-room facility that could be a division-wide resource and have the potential for nucleating cross-division collaborations. The Nanomechanical Properties Group is developing an impressive suite of techniques to measure mechanical, adhesion, and strain properties at multiple length scales. The prospect of achieving single-grain response and of extending these experiments to other temperature and mean pressure states is exciting and could revolutionize understanding of the mechanical response of all condensed matter.

The Security Technologies Group focuses on measurement science as it applies to body armor, the detection of hidden weapons using millimeter-wave imaging, and more exotic technologies such as those for the detection of individuals buried in rubble or obscured by walls. The work of this group has a strong focus on Department of Justice needs and also benefits from interaction with the Army Research Laboratory (ARL). The body armor study combines ballistic testing with measurement of aging (hydrolysis) effects of the relevant polymers, fabrics, and composites. The ballistic testing uses a dedicated indoor firing range with a configurable, handgun-scale, remotely operated breech. A novel, very-high-resolution laser velocimeter determines projectile velocity. The quality of work is very high, benefiting from the great variety of expertise at NIST, ranging from textiles to optics. However, the testing facility itself is not unique, and experiments of equal caliber might be conducted with ARL or other research associates.

Opportunities and Challenges

The Nano Materials Research Group and the Materials for Energy and Sustainable Development Group are doing high-quality research and yet are relatively small players in very big fields that are seeing major investments around the world; one implication of this situation is that the groups will need to specify the niches in which they are likely to make the greatest contributions and to adjust their niche as developments warrant. The Security Technologies Group appears to be without clear cross-cutting roles. While this group could benefit from the leading instrumentation available in the other groups within the MMSD, these partnerships are in the very early stages of development, and so there is much room for growth.

The Surface and Trace Chemical Analysis Group, which works closely with the Security Technologies Group, is at the forefront of ion- and photon-based imaging and spectroscopy, is extraordinarily well equipped across the board, and is recognized as being at the forefront of such techniques. One exception to this statement is the 3-D atom probe, which is an instrument to which the MMSD has come rather late in the game. Nevertheless, the 3-D atom probe is a field in which quantitative understanding of data and standards is needed, so there is opportunity for significant impact.

The Synchrotron Science Group has one of the leading materials-characterizing facilities in the world and runs an effective user facility, considering performance metrics that include number of papers published (90-100 every year from facility users), number of high-profile papers, and number of users (more than 100 industry and academic researchers). The Synchrotron Science Group is performing at the highest level. Its development of soft x-ray analysis and imaging is extraordinary. It has been developing unique synchrotron techniques. This research effort comes at a time of transition—the closing of the National Synchrotron Light Source (NSLS) I and the commissioning of NSLS II. During this transition, 16 spectroscopy beamlines at NSLS I will be reduced to 3 in NSLS II; the MMSD team will be the lead for 2 of these. This transition will cement the MMSD Synchrotron Science Group's position at the forefront of x-ray characterization of materials, which will be critical to the success of NSLS II.

When the NSLS II is commissioned later this year, its new beamlines—spectroscopy soft and tender (SST)1, SST2, and the beamline for master measurements (BMM)—will have a number of unique capabilities. The three beamlines will be designed for high throughput to optimize new materials discovery; they are well positioned to contribute to the Materials Genome Initiative. The combination of workhorse techniques for characterizing materials with new developments in spectroscopy and spectromicroscopy techniques is impressive. The soft x-ray emission and near-edge x-ray absorption fine structure (NEXAFS) technique is very powerful and shows the power of leveraging the capabilities of NIST at Gaithersburg, Maryland, and Boulder, Colorado, in order to develop and implement the microcalorimeter array for detection. The hard x-ray photoelectron spectroscopy (HAXPES) full-field magnetic projection microscope is also an exciting advance. The transition from NSLS I to NSLS II required a recent investment of $8 million. The current institutional services (IS) tax imposed on all expenditures that started in fiscal year 2013 constitutes a particular burden for synchrotron activities. It would be a shame if this highly collaborative and important program were damaged due to recent changes in overhead policy.

Overall Assessment of Technical Programs

The dispersal of MMSD scientists across eight buildings in Gaithersburg and a separate National Laboratory makes it challenging to grow a coherent division. Cross-cutting thrust areas, such as the Materials Genome Initiative, are of secondary interest to most of the scientists, but much of the work in all the groups fits well into the MML thrust areas. It is too early to see whether the decades of preexisting collaborations are being enhanced by the new organizational structure. Certainly there are many opportunities to build new collaborative efforts. There are, however, concerns among the staff about the loss of opportunities for collaborations with entities outside NIST because of increasing budgetary, administrative, and legal constraints. Overall, the technical programs in the MMSD vary from world-leading centers to groups in need of improvement and better integration to form a more coherent division.

PORTFOLIO OF SCIENTIFIC EXPERTISE

MMSD staff are scientific leaders in the areas of x-ray methods, electron microscopy, and surface analysis. The Brookhaven NSLS group is noteworthy for its leadership and innovation in synchrotron spectroscopy and imaging methods.

Expertise in atomic structure and thermodynamics supports the development of databases on material structure and phase diagrams and x-ray diffraction and spectroscopy, which directly support the division's core mission of supporting industry through the development and dissemination of standards.

The development of new micro-indentor instrumentation exemplifies the division's historical expertise in building state-of-the-art instrumentation. The microscale stress–strain measurement capability is innovative and extends the division's expertise in strength and failure in materials. The work on nanoparticle separation and high-throughput analysis is very good, and the MMSD has established unique expertise in this area. However, it is not evident that the MMSD nanoparticle expertise is equally strong in all areas of this broad and rapidly expanding field. The measurement of thin-film structure and chemical characterization and the measurement of thin-film thermodynamics are outstanding. The more applied research is on thin films, and related applied research in the energy area is good and on a par with that in academia. The junior staff are excellent and reflect the success of the National Research Council postdoctoral program to attract energetic researchers to the division. They appear very happy with the research environment and are well mentored by the senior staff, but they have expressed concern about the increasing demands of paperwork and restrictions on travel.

Because of the dearth of technicians, Ph.D. scientists do routine tasks like computer system maintenance, which is a poor use of their skills and resources. There is a strong need for technician support, particularly for information technology support, in view of the mandate to make public all data. The current computer infrastructure is not equal to the task.

In the Microscopy and Microanalysis Research Group and in the Surface and Trace Chemical

Analysis Group there is an outstanding blend of senior and younger scientists and engineers who are excited about the science they perform and the instruments they develop and who are creating innovative instrumentation and needed SRMs, software, and comprehensive reports.

The Synchrotron Science Group also has an outstanding blend of senior and junior scientists. The group leader has more than 20 years of experience with synchrotron techniques and interfacing with industry. The group delivers a great deal of output given its limited size.

The Materials and Structure Data Group might benefit from increased collaboration with the Brookhaven Synchrotron Science Group.

The Security Technologies Group has unique expertise in millimeter-wave detection and imaging. However, the body armor research does not connect well with the core strengths of the MMSD, which emphasize atomic scale characterization and thermodynamics.

ADEQUACY OF FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

Overall, the ratio of equipment capital to human capital is high, consistent with the MMSD mission to pursue state-of-the-art metrology, microscopy, and spectroscopy. Within the division, there are a number of capabilities to measure and characterize materials that are unique, either to NIST or to the broader international research community.

The test bed for trace explosives supports the deployment of screening technologies to NIST gates and to the training of law enforcement officers. State-of-the-art microscopy and microanalysis instrument suites cover elemental, compositional, and phase characterization of particle and thin film sample systems that are relevant to national security and support collaborative research efforts within the division and across NIST. Unique materials formulation and fabrication facilities address the needs of outside agency customers. Developed capabilities also include a novel passive millimeter-wave imager and test bed; a suite of gravimetric materials deposition printers for standards production; a suite of custom-designed nano-indenters; and unique synchrotron end stations and spectro-microscopes. A NIST-developed measurement system combines a modified electrospray-differential mobility analyzer coupled to an inductively coupled plasma mass spectrometer; this unique capability allows selection of particles of a specific size, with sub-nanometer resolution, counts the particles and analyzes them for core and surface elemental composition. The partnership with Brookhaven is of the highest quality and deserves continued support. The MMSD is also pushing the limits of techniques such as 3-D atom probes, nano-indentation, secondary-ion mass spectrometry (SIMS), and electron microscopy and microanalysis.

Despite funding issues, the Microscopy and Microanalysis Research Group has been highly successful in building a set of scientific instrumentation that is within the top 10 in the world, including top-of-the-line commercial instruments and unique inventions, which are used to address hitherto-unanswerable materials questions. The group is well staffed, well led, well equipped, doing outstanding research, providing globally recognized SRMs, and addressing the industry and national security needs that are brought to it.

In the Nano Materials Research Group, the portfolio of scientific expertise, the adequacy of facilities, equipment, and human resources, and the dissemination of outputs are all similar to those just described for the Microcopy and Microanalysis Research Group. High-quality research is being performed in some very select fields, but the biggest challenge for the Nano Materials Research Group is that its thrusts and goals represent only a small portion of global interests within a huge field of great international interest and importance. It is difficult to be recognized as a world leader when the overall scale of many other nano-materials research groups is so much broader and deeper.

The Surface and Trace Chemical Analysis Group has an impressive suite of commercially based instruments, including secondary ion imaging and tomographic atom probe analysis coupled with laser excitation of surface atoms.

In the Synchrotron Science Group the beamlines currently being supported include the current beamline X23A2 (4.7 to 32 keV) x-ray absorption fine structure spectroscopy (XAFS); beamline U7A

(0.175 to 1.3 keV) near-edge x-ray absorption fine structure spectroscopy (NEXAFS); and beamline X24A (0.7 to 5.0 keV) hard x-ray photoelectron spectroscopy (HAXPES) at the NSLS I. The energy range covers the entire periodic table, which enables the study of a broad range of technological materials, including inorganic and organic semiconductors, photovoltaics, self-assembled monolayers (SAMs), biological and environmental materials, batteries, catalysts, fuel cells, polymers, superconductors, ferroelectrics, and ferromagnets. This facility provides unique opportunities for collaborative research within the MMSD, with MML personnel across divisions (including the Boulder, Colorado, facility), and with the broader user community, including numerous industrial partners.

Across the MMSD, the internal assessment of output seems satisfactory and recognizes the different expectations placed on individuals, but some staff expressed concern that these division-level assessments were not always understood at the MML level and above. For example, an instrument developer who takes years to build a unique tool that results in a handful (or less) of publications during that time, appears to be at a disadvantage for promotion, merit pay, fellow status, and other forms of recognition compared to more academically oriented researchers whose H index in high-impact journals is immediately recognized.

The scientific staff in the MMSD expressed an impression that the group is disproportionately impacted by the IS tax because it is heavily reliant on equipment with service contracts. The IS tax also affects contracts with academic associates. It adds to indirect costs at university and industry partners, reducing the value of these partnerships. MMSD management needs to examine with MML management whether this overhead structure is achieving its aims and needs to communicate with staff about why the structure is in place, how it benefits the groups, and how perceived concerns can be addressed. The fact that recent capital investment rates are well below depreciation rates is another challenge. Given these trends, the equipment/scientist ratio is at risk of decreasing significantly, which would be counterproductive to the mission of the division. There are, then, concerns about the division's ability to maintain current service contracts and buy new expensive instruments that will keep the MMSD at the scientific forefront. The possibility that the central MML budget might be a source for such new instruments needs to be communicated more clearly to the bench scientists who are unaware of this option.

Procurement and legal issues are perceived by some staff as day-to-day threats to carrying out the missions of the groups in the MMSD. There is also some concern about the lack of travel opportunities for junior scientists, although the situation appears better than at some other federal facilities.

The Securities Technologies Group lost $2 million of its $3.8 million scientific and technical research and services (STRS) budget when the reorganization of the MML occurred. This cut, together with the IS tax, inhibits the group's ability to engage in meaningful collaboration with academic associates. Legal delays have cost the group a motivated industrial partner. If the Securities Technologies Group does not receive sufficient support to meet its technical goals, its portfolio might appropriately be integrated into the portfolios of other adequately resourced groups.

In general, the facilities are adequate for the division's mission, with the principal difficulty being the dispersal of the division in buildings across the NIST site. There appears to be no imminent solution to such scattered facilities, and so the growth of collaboration between cross-cutting thrusts might prove less than ideal. Scientific instrumentation is generally of extraordinary quality across many of the groups. Some pieces of equipment are unique and some world leading, matching the quality of the staff. The human resources are highly accomplished, collaborative, and effective in their equipment usage. Common to all groups, there are opportunities for more communication with MML leadership on issues such as procurement, the IS tax, and travel processes.

DISSEMINATION OF OUTPUTS

The MMSD is highly effective in disseminating its program output. It has a successful publication record that corresponds to roughly one publication per person per year. This may appear modest compared to other top-tier research institutions, but the unique mission of the MMSD yields output in many areas other than publication. The division's publications are in a broad range of fields, reflecting its diverse research activities, and over the past year have included publications in high-impact journals such as *Nature Materials*, *Nano Letters*, *ACS Nano*, *Advanced Energy Materials*, *Advanced Functional Materials*, *Chemistry of Materials*, and *Small*. Many of the papers are coauthored with researchers outside NIST; this indicates successful collaborations.

Patenting is secondary to many other success metrics for almost all MMSD staff researchers, and there were only two division patents in the past year.

The MMSD works closely with industrial partners. There have been three cooperative research and development agreements (CRADAs), including one with the Dow Chemical Company on synchrotron materials characterization and one with Intel-ENIAC on emerging nanoscale interface and architecture characterization. These CRADAs are important contributors to the division's research portfolio.

The division has developed three commercial swipe technologies, and three printer systems have been commercialized. The division sells approximately 1,700 reference materials units per year of almost 80 different types. The total revenue is about $300,000 per year. These materials cover a variety of needs, including x-ray diffraction characterization and calibration, particle size (including nanoparticle sizing), glass viscosity, refractive index, surface area, and chemical composition. About 20 percent of the customers are from academia; 20 percent from state, local, and federal governments; and 60 percent from industry. Examples include SI-traceable SRMs for calibration of varying diffraction measurement methods. This product is highly effective, and there is hardly an x-ray diffractometer in the world that does not use the NIST standard. Roughly a third of new instruments sold worldwide include a NIST standards diffraction package.

The MMSD also provides SRD covering crystallographic and structural information, phase diagrams, surface spectroscopy, ceramic properties, and x-ray and image analysis, all of which are used worldwide. These standards are a major resource for researchers, and the MMSD expends enormous efforts to incorporate image processing and theoretical/statistical methods within materials databases to expedite experimental data standardization and evaluation.

MMSD representation on standards-setting committees is outstanding and is a significant output of the division. Twenty-eight MMSD staff members actively participate on committees in 125 international standards organizations (primarily ASTM and ISO). This participation includes standards committee leadership, with the following subcommittee chair positions: ASTM International Committee E56 on Nanotechnology; ASTM F12.60 Committee on Controlled Access Security, Search, and Screening Equipment; ASTM F23.25 Committee on Ballistic Hazards; ASTM E54.01 Subcommittee on CBRNE Sensors and Detectors; IEC TC85 (PT62792, MT18, WG22) Committee on Measuring Equipment for Electrical and Electromagnetic Quantities; and IEEE TC10 (subprobe standards, subpulse technology) Subcommittee on Waveform Generation, Measurement, and Analysis.

The MMSD has generated for other agencies significant outputs that for security reasons are not included in its list of publically available publications. These include 115 reports of analysis, 15 reports on the status of projects, and 4 written and 3 oral research and development reports that summarize the status and outputs of projects.

Since the beginning of 2014, the division has conducted significant outreach and training for visitors, including 72 tours for 485 hosted visitors. The division has hosted more than 1,500 visitors since 2009.

OVERALL ASSESSMENT

The strong collaboration across the groups that existed before the formation of the MMSD has continued. The management expressed its commitment to making the division more than the sum of its parts, but this remains a challenge. The MMSD appears well managed, with an enthusiastic cadre of administrators and active researchers who perform high-quality science. The research activities are nicely balanced between basic research, where the primary output is peer-reviewed publications, and technical programs that serve the standards mission of NIST. While improvements in the demographic diversity of the division are needed, there is strong evidence that the female leaders are well respected and contribute fully at the leadership table. The morale of staff, from postdoctoral researchers through emeritus fellows, appears high. The MMSD is successfully maintaining a culture that fosters loyalty, partly because staff have the opportunity to focus primarily on research. Overall, the quality of the research in several traditional standards-related areas is world leading. For example, the Microscopy and Microanalysis, the Surface and Trace Chemical Analysis, the Materials Structure and Data, and the Synchrotron Science groups are all at the top of their fields in the United States, have been recognized as such by their peers for many years, and are acknowledged internationally as being among the top 10 in their fields worldwide. In its chosen niche area, the Nano Materials Group is also world leading. The Materials Structure and Data Group is the acknowledged source of phase diagram and crystal structural information around the world. The Microscopy and Microanalysis Group and the Surface and Trace Chemical Analysis Group have long been recognized as the organizations that set the world standards for quantitative electron imaging, x-ray analysis, and secondary ion imaging and analysis.

FINDINGS AND RECOMMENDATIONS

Current expenditures for the acquisition of new equipment and for maintaining existing facilities are inadequate to support the high-quality programs. This is a particular challenge for the Synchrotron Science Group, which is a jewel in the crown of the MMSD.

Recommendation: The Materials Measurement Science Division should, to the extent possible, ensure that the funding for top-tier instrumentation is commensurate with the division mission and the structure of the institutional services tax.

The quality of the junior staff is excellent. It reflects the success of the National Research Council postdoctoral program in attracting young talent to NIST and also reflects the success of senior staff and management in mentoring the new hires.

Recommendation: The Materials Measurement Science Division should continue support for the National Research Council postdoctoral program and should explore ways to continue to lower barriers for external collaboration and travel to professional meetings, so staff may build international standing.

The researchers reported that they are increasingly burdened by administrative duties (e.g., procurement and legal processes) and responding to unfunded mandates such as the Digital Accountability and Transparency Act (DATA).

Recommendation: Materials Measurement Science Division management should continue efforts to open doors between the administrative offices and researchers and to streamline purchasing and legal processes.

The division's eight well-established groups are spread across multiple buildings. For this reason, the researchers tended to identify with their particular group rather than with research thrusts. The development of a more coherent division is slowed by this distribution of groups and facilities across multiple buildings.

Recommendation: The Materials Measurement Science Division management should

continue efforts to improve cohesion and collaboration among the groups and increase the importance of cross-cutting thrust activities that magnify the many outstanding strengths of the division.

The core strength of the MMSD is its very long-term investment in basic research and the iterative development of new instruments to advance measurement science. Over the past decade, a shift to short-term, customer-driven research and responses to unfunded mandates are eroding this long-term strategy and are promoting more short-term, applied research in areas where the MMSD is less competitive compared to academia and other national laboratories.

Recommendation: The Materials Measurement Science Division should encourage long-term basic research.

7

Materials Science and Engineering Division

The Materials Science and Engineering Division (MSED) consists of 52 permanent technical staff members, 19 National Research Council (NRC) postdoctoral fellows, 2 NIST fellows, and 102 NIST associates. The division is located in Gaithersburg, Maryland. It was formed by combining the Metallurgy Division and the Polymers Division of the former Materials Science and Engineering Laboratory. A portion of the Polymers Division, the Biomaterials Group, was assimilated into the new Biosystems and Biomaterials Division. The mission/function statement of the MSED is as follows:

> The Materials Science and Engineering Division provides the measurement science, standards, technology, and data required to support the Nation's need to design, develop, manufacture, and use materials. In partnership with U.S. industry, other government agencies, and other scientific institutions, the division develops and disseminates measurement methods, theories, models, tools, critical data, reference materials, reference data, standards, and science underpinning the Nation's materials science and engineering enterprise. These activities foster innovation and confidence in measurements needed to advance technology and facilitate manufacturing in industrial sectors such as energy, electronics, transportation, and the environment." [1]

The MSED consists of five technical groups and the division office. The groups are the Thermodynamics and Kinetics Group, the Functional Nanostructured Materials Group, the Polymers and Complex Fluids Group, the Functional Polymers Group, and the Mechanical Performance Group. In addition, the division plays a significant role within NIST for two cross-cutting programs: the Materials Genome Initiative and the additive manufacturing program within the NIST advanced manufacturing initiative.

ASSESSMENT OF TECHNICAL PROGRAMS

Accomplishments

Notable work of the division includes developing new data sets and advanced models for the properties of nanostructured inorganic materials; establishing the nSoft Consortium, whose goal is to advance and transfer neutron-based measurement methods for soft materials manufacturing and which merits consideration by other MML divisions as a means of collaboration with industry and academia; the unique cruciform multiaxial mechanical test facility, incorporating a high-rate servohydraulic frame; a critical dimension measurement by the critical dimension small-angle x-ray scattering (CD-SAXS) technique for metrology of thin films in semiconductor manufacturing, reducing times for data acquisition from tens of hours to tens of seconds; a unique industrially scalable method for separating conducting and

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[1] NIST Material Measurement Laboratory, "2014 National Research Council Assessment of the NIST Material Measurement Laboratory-Read-Ahead Materials," Gaithersburg, Md., June 2014.

semiconductor carbon nanotubes (CNTs); and new energy storage materials, such as next-generation electrodes for high-capacity Ni-MH (nickel-metal hydride) batteries.

Materials Genome Initiative

The NIST portion of the national Materials Genome Initiative (MGI) effort, which is less than 2 years old, is focused on developing new methods and tools that would allow integration of data, informatics, computational models, and experimental results. NIST hosted the first customized data repository for the materials community, which allowed linking of data between files, including metadata. First focus is on phase-based materials property data, allowing customers to contribute to and search for data on the NIST Internet site. Work at the MSED has been started on improved methods of data curation and ontology, enhancement of the data repository, and development of a variety of computational microstructural and molecular-based modeling tools. The goal of MGI is to reduce by half the cost and time to market of a new material. Consequently, the project requires establishing interfaces with other NIST divisions, other government agencies, and appropriate industrial sectors for data accumulation that are in the public domain and identification of which NIST deliverables would be most useful in pursuit of the MGI goal.

Additive Manufacturing Program

The newly established additive manufacturing program is off to a good start—the team has been formed, and the effort has been focused on filling a gap in the knowledge base for additive manufacturing. As a first effort, understanding the microstructural evolution of as-deposited metallic materials, which have relatively poor properties, into a high-strength structural material is essential. A similar effort will be initiated for organic polymeric materials. An important output of this effort involves understanding how the specifications of the starting material and machine processing parameters relate to a material's performance, including what defects are added to the microstructure during processing. This understanding will allow this new manufacturing technology to advance much faster.

Thermodynamics and Kinetics Group

The Thermodynamics and Kinetics group investigates the thermodynamics, kinetics, phase transformations, microstructure evolution, and properties of materials of technological interest. The group possesses computational assets such as computer servers, storage, and workstations and has been working on a variety of computational codes. In addition, it has access to a wide variety of computational tools and techniques, such as density functional theory (DFT), for prediction of material characteristics, leveraging data from a large number of known materials. The group's early entry into the data repository field is essential for the success of the MGI. Utilization of thermodynamic and kinetic laws and models for prediction of microstructures and phase transformations and their relations to properties has been a long-standing challenge to materials scientists, solid state physicists, and chemists. The staff has begun to address the challenge of designing new materials based on knowledge derived from experimental observations and modeling. Some of the experimental facilities accessible to the group are state-of-the-art and could be utilized on focused material design challenges, although the group is currently largely focused on metallurgy. DFT computational techniques have benefit for one-dimensional structures (e.g., graphenes and nanotubes). DFT utility for 3-D structures is more limited and requires integration with other computational tools.

Functional Nanostructured Materials Group

The Functional Nanostructured Materials Group works at the nano- and microscales to develop measurements and models that correlate chemical, electrical, and magnetic properties of nanostructured inorganic materials to their microstructure and processing. They are conducting excellent programs in magnetic materials, energy storage, and nanowires. Work is of high quality, and the equipment matches its research effort. Collaboration with leading institutions such as Carnegie Mellon, General Electric, and Seagate Technology LLC to develop nanomagnets for storage and post-CMOS complementary metal-oxide-semiconductor integration holds high promise for success. The effort on electrochemical processes for deep trench isolation of through-silicon vias is industry-driven and important to advances in the semiconductor industry. Researchers addressing functionalized magnetic nanoparticles, thin-film and bulk magnetics, nanowires, advanced batteries, and challenges in understanding electrochemical processes are on the cutting edge of technology. The development of new energy storage materials for high-performance batteries is another area of great importance, and the group has demonstrated good progress. Because of its technological importance, this area is being addressed by researchers worldwide. It would be of value to maintain a close watch on progress in other laboratories. The group's characterization of a next generation of multicomponent, multiphase materials for electrodes in high-capacity Ni-MH batteries is an outstanding accomplishment.

Polymers and Complex Fluids Group

The Polymers and Complex Fluids Group investigates soft materials, such as multiphase fluids, gels, and composites, and their constituent components. Composites are a materials class of considerable current scientific and technological interest. For electrically conductive composite materials, this group has developed noncontact techniques for measuring conductivity in nanotube polymer composites employing microwave radiation, a technique that is very useful albeit not unique. Matrix interface interactions are a key aspect of high-performance polymer composites, and the group has attacked the issue of characterizing the interface using fluorescence resonance energy transfer (FRET) techniques, which are well suited to such imaging studies because of the relatively short-range nature of the interactions. This provides an imaging tool for composite interfaces if appropriate dyes can be incorporated, and the approach only requires a fluorescence microscope. Fluorescence and atomic force microscopy (AFM) have been coupled through opposite-side viewing to produce fluorescence images of AFM-imaged nanostructures. This is a clever combination that could be used to study shape and structure in nanostructures. The application of the techniques for studying nanostructure composites could be particularly useful.

This group seems focused on innovative tool integration and plans on coupling Raman and other spectroscopic methods with realistic flow and deformation environments for nanoscale, in situ measurements of material structure. These are first-rate efforts to couple multiple spectroscopic and mechanical probes to study the mechanical behavior of nanostructures and structures under stress. The study of mechanical properties under high strain and extreme conditions is of substantial technological interest. The performance of advanced materials under extreme conditions is critical for many applications, and fundamental understanding is critical for the design of new advanced materials. The collaborative effort with the Mechanical Performance Group links the mechanical performance understanding of hard and soft materials, such as the study on Kevlar fiber stiffing at high strain and the work on the optimization and standardization of ballistic clay.

The group has emphasized the study of viscous flow of solutions and heterogeneous mixtures in confined dimensions. The study of size and shape of heterogeneous and homogeneous interacting additives in fluid solution and microfluidic studies is important for biomedical applications, including delivery of macromolecular therapeutics. This understanding is critical to programs like NIST on a Chip (NIST precision measurements and physical standards that are miniaturized and deployable in customers' tools and products). There are strong connections with a number of drug and pharmaceutical companies, including MedImmune, which maintains an assignee on site to leverage the applications. For particles, velocity sectors in confined flow have been studied spectroscopically by evanescent wave activation. This is a broad-based effort in flow hydrodynamics and surface-fluid interactions with technological applications, particularly in the biomedical area.

The project for macromolecular characterization leverages the MSED's considerable expertise on x-ray and neutron scattering and on reflectivity. The former are critical to characterization of macromolecules in solution and the latter can be applied to surfaces. The dynamic behavior of materials anchored to surfaces is critical to microfluidics, particularly for biomedical applications where surface shape and dimensional changes can influence flow and capture dynamics. This group is leveraging the NIST expertise in measurement and modeling and the NIST facilities (e.g., n-Soft) for high-energy reflectivity as a probe of surface structure.

The project on particles, tubes, and colloids has academic and industrial support. It directly addresses a key barrier to implementation of carbon nanotubes into electronic devices—the purification of the nanotubes, particularly the separation of conducting and semiconducting nanotubes using a process that could be scaled industrially. The two-phase extraction process developed in this group may solve this issue and produce a separation process that is scalable. It has led to a patent that has generated considerable licensing interest. The studies on CNT separations and CNT properties have led to more than 15 publications in a relatively short period.

Functional Polymers Group

The Functional Polymers Group addresses the electrical, chemical, and magnetic properties of nanostructured inorganic materials, including metals and semiconductors, as related to their microstructure and processing. It focuses on three general themes: transport membranes, printed and flexible electronics, and dimensional metrology. A key goal of this group is the development of a portable, stable, bright x-ray source (perhaps liquid metal jet anode) to overcome the major remaining issue hindering industrial adoption of CD-SAXS as a metrology tool. The group has made steady progress and is tied in to pattern modeling efforts with block copolymers, which may be the patterning technique of the near future. Its connection with the University of Chicago in modeling will be very helpful in this regard. The cornerstone of organic electronics rests on cost, ease and control of processing, and manufacturability. Consequently, the group's efforts in printed and flexible electronics are focused on in situ determination and control of the morphologies of photovoltaic materials and organic transistors in roll-to-roll or blade-coated processes. This type of monitoring is critical, because the optical and electronic properties are so strongly tied to polymer morphologies. A variety of optical, scattering, and diffraction techniques have been adapted to the study of in situ evolution of crystalline and amorphous domains in continuous coating processes. The recent acquisition of a slot die roll-to-roll coating apparatus is likely to greatly facilitate the integration of in situ metrology. The importance of this type of information is confirmed by endorsement from more than 10 academic and industrial partners.

There is a significant research effort in the area of membranes, with a unifying theme of transport in polymer materials such as ion, electrical, proton, and water. These efforts are highly collaborative, particularly in the area of new materials, and utilize the group's strengths in characterization and measurement, leveraging common techniques for the benefit of each program. A focus on solid electrolytes is appropriate, given the stability issues for liquid electrolytes in various applications. The program studying aspects of water in membranes (penetration, distribution, occupancy, volume, and diffusivity) is quite extensive, utilizing the MSED's characterization expertise in thin films (x-ray scattering and reflectivity and neutron scattering and reflectivity in deuterium oxide [D_2O]) to study the matrix polymers and their specific long- and short-range interactions in model membranes and constrained films; the formation of ultrathin film membranes prepared using automated layer-by-layer assembly; and analysis of the water content and diffusivities as a function of systematic charges in membrane chemical structure. The use of poromechanics in water-containing films to study the diffusion of water displaced by mechanical stress is innovative and has great potential. Accurate estimation of solubility and diffusion coefficients for water is key to membrane performance for desalinization.

Mechanical Performance Group

The Mechanical Performance Group performs a significant portion of mechanical testing at NIST, including testing materials under extreme environments, but it is focused primarily on metals, which is a legacy of the merger of the polymers and metallurgy groups into a single division. The automotive lightweighting project is a particularly interesting initiative. Given increasing pressure for accelerating mileage standards in the automobile industry, the focus on high-strength steels, metal alloys, and polymer composites is inevitable. The requirements for material strength, resilience, and safety, coupled with cost and manufacturability, are a significant challenge to the domestic and international automotive industry. The approach of the automotive industry to new material development and testing involves identifying a material, fabricating it into a component, and testing it in a vehicle crash test. While this provides the ultimate test, it is an expensive, time-consuming way of surveying potential materials candidates.

The automotive lightweighting project is addressing this need by developing testing instrumentation with in situ analysis capability that produces data that can be used by advanced computational design tools. The cruciform biaxial stress and strain testers with in situ optical and x-ray monitoring are unique. They have produced some very useful data on magnesium sheet alloys and seem applicable to testing a wide range of relevant metallic alloys and polymer composites. This information will greatly aid automotive designers by providing critical data required by sophisticated predictive tools, which are expected to be widely utilized in the future. The project also seems to be well connected to the automotive industry and to the regulatory agencies. The fact that industrial customers have been participating in developing the requirements for the group's capabilities and are widely using this facility is seen as a validation of its skills and the importance of its work.

Moving forward, the group is focused on developing metrological foundations for nanomechanics utilizing nanoindentation and submicron diffraction for nanoscopic measurements of strain tensors, supported by DFT modeling and simulations. Given the current focus on nanomaterials and nanotechnology, this is a useful thrust that fits in well with the addition, in 2014, of the nanomanufacturing initiative. The development of nanoscopic characterization techniques such as tomography, microdiffraction, and imaging will be critical to this initiative and positions the group to participate in and contribute to the initiative.

The group's capability for determining mechanical properties under extreme conditions and high strain is impressive. The research equipment has been used to characterize high rate deformation characteristics, which are very difficult to measure accurately, in both soft materials (Kevlar fibers) and metals. The effort in soft materials is a collaborative project with the Polymers and Complex Fluids Group.

Opportunities and Challenges

The Materials Genome Initiative (MGI) is a challenging and ambitious effort within the national MGI effort, and it will require years of consistent and deliberate efforts to identify and close gaps, develop experimental and theoretical program plans, and complete, in the near term and long term, projects that are built on MML strengths and are useful to the NIST users as well as external customers. NIST is the singular institution to focus on materials data informatics. There are no accepted ontology tools for the broad expanse of materials, and the project is just beginning to assess what is necessary in this area. Until a detailed project roadmap is constructed with input from the user community, it will be challenging for the program to request additional out-year funding.

Additive manufacturing, and 3-D printing in particular, is a rapidly emerging manufacturing process capable of producing rapid prototypes to enable compressing component design cycles, and it is also being extended to the manufacturing of difficult-to-produce high-performance components. Much of the recent activity involves producing metallic components with usable structural properties; the research has been largely trial-and-error, so this project does fill a gap. Understanding how an as-deposited microstructure can be transformed into a high-performance structural material, taking into account processing conditions and starting material specification, would be of great benefit to industry. It will also accelerate efforts that are developing new material chemistries to more fully exploit the capabilities of additive manufacturing. Because there already is a substantial industrial effort in additive manufacturing, the MSED team will have to get to know the stakeholders and use these interactions to prioritize its efforts and identify the best means to disseminate the results of its work.

The Thermodynamics and Kinetics Group has taken on the task of collecting and storing data regardless of the format in a form that is easily searchable and rapidly accessible; this task is beyond the capability of this small team. Success will require the collaboration and coordination of resources with the new Office of Data and Informatics, which is tasked with helping researchers tap large, information-rich sources as well as providing an interface with the NIST Information Technology Laboratory for data curation and development of a materials-based ontology. Such cooperation will be essential for the establishment and utilization of repositories associated with the MGI. NIST has expertise in assembling and maintaining repositories for data in areas such as mass spectrometry and interatomic potentials, but repositories for the MGI initiative are far more challenging.

Utilization of thermodynamic and kinetic laws and models for prediction of microstructures and phase transformations and their relations to properties has long been a challenge to materials scientists, solid-state physicists, and chemists. An admirable goal of this group is applying its expertise to create a user-friendly interface for computation and modeling that helps tailor computational method and parameters to the properties of interest for metals, soft materials, and CNTs. The group is heavily focused on DFT techniques and their application to metals, alloys, and metal oxides. One of the challenges in meaningful DFT methods is the plethora of choices for matching the most appropriate method to the particular application. The group could help to address this challenge by serving as a repository of expertise for the uninitiated, because DFT techniques are usually the domain of the sophisticated user. More connection of this group to those in other groups working with soft materials modeling and simulation would be worthwhile. Creation of a broad-based focus group involving relevant researchers across the division could be helpful in uniting disparate efforts.

The Functional Nanostructured Materials Group has excellent programs in magnetic materials, aspects of energy storage, and nanowires. Because these efforts are all of high scientific and commercial interest, there is a significant amount of ongoing research in these areas outside NIST. Collaboration with other institutions is important to ensure that the MSED is focusing its resources in the most useful areas.

The Polymers and Complex Fluids Group identified computational capabilities as a strength, particularly in the area of soft materials, but little evidence of its impact on existing programs was presented. This is a key topic noticeably missing from the Thermodynamics and Kinetics Group, which is focused on DFT techniques and metallic and inorganic materials. Together the two groups could provide reasonable computational coverage over the range of materials of interest division-wide. The fluorescence resonance energy transfer (FRET) interface imaging approach has great potential, but it has not been demonstrated to be practically useful. Metallurgy and polymer teams seem to be working independently, with the exception of high-strain-rate testing, where collaboration is evident. Two new efforts exhibit considerable promise. A project on polymer processing and rheology, initiated in 2014, meshes with the in situ studies of materials under extreme conditions. The goal is to study polymer structural changes during processing. Such in situ information could be essential for optimizing applications such as inkjet printing of polymers for electronic applications and injection molding of polymers. Although the collaborators at this early stage are primarily academic, ExxonMobil has recognized the importance for polymer film and shape processing. The second project, the separation of surfactant-coated CNTs by specific biomolecule recognition, is an extension of the ongoing work to identify practical means to quickly and inexpensively separate different types of nanotubes.

The Functional Polymers Group has focused on membrane separations as a very important area with significant commercial applications; for this reason, the scientific challenges are also being investigated by many others. The MSED has the opportunity to stimulate scientific thinking and help guide the measurement science used by the external groups in the many areas of industrial importance for membranes, not limited to water purification. There is an opportunity to unite disparate applications within the group with common metrology methods, such as what was effectively done for membranes. The effort to develop a portable, stable, bright x-ray source to make CD-SAXS an industrially viable metrology tool is now particularly understaffed.

The principal effort of the Mechanical Performance Group is related to mechanical properties of metallic materials, with soft materials a distant second priority; the only polymer-related effort was the project on measuring the high strain behavior of fibers. There are numerous pockets of soft materials mechanics work scattered throughout the division that would benefit from collaboration by the mechanical performance experts in this group. The cruciform biaxial stress and strain testers with in situ optical and x-ray monitoring are unique, although it may be duplicated in other locations in the future. This equipment has already produced some very interesting data on magnesium alloys, and there are plans for testing a wide range of relevant metallic alloys. This technique may not be limited to metallic materials: it could also be considered for testing other materials, such thermoplastic composite materials, without compromising the group's support for metallic materials. Increasingly, advanced material structures place demands on the design of composite materials, which include metal, polymer, and ceramic matrix composites and composite coatings for high-temperature application.

Ceramic composite materials are being applied in aerospace and other industrial sectors, such as solar energy. High-temperature testing of these materials is a challenge, especially long-duration, strain-controlled, low-cycle fatigue testing, because the durability of the testing equipment is problematic, and contact gauges to measure displacement are not useful. Development of suitable testing equipment and related standards is evolving, and experts at the MSED could add needed expertise.

Overall Assessment of Technical Programs

This newly formed division (less than 2 years old) has had an encouraging start. The technical program portfolio is robust, has major accomplishments, and is strongly linked to the MML mission. For the most part, the work is at the cutting edge, in some cases pointing the technical community to innovative solutions to complex problems. A key challenge is to effectively integrate the disparate technical efforts within the division into a seamless and uniformly productive unit, because they are addressing highly diverse areas of research and standardization for a wide spectrum of materials and processes. This combination of metallurgy and polymers is not common in academia and industry at this scale. There are meaningful projects under way that entail synergy between the polymers experts and the metallurgists, although this is still evolving.

The newly initiated effort to construct a strategic plan for the MML will help in the assessment of additional opportunities for research within the MSED and will provide a basis for balancing the resources and efforts across the groups. Constructing a strategic plan and the roadmaps that likely will result from it is a substantial effort that would benefit from involving most, if not all, of the technical experts within the division.

Support for new cross-cutting programs at the expense of current ongoing programs can be a challenge of which the research groups are well aware. There is evidence of satisfaction in working on a cross-cutting program; this is a testimony to the division leadership's success in communicating the importance to the nation of supporting these initiatives.

PORTFOLIO OF SCIENTIFIC EXPERTISE

The MSED has an impressive array of scientific expertise that is suitable to address the advanced technology challenges that the division undertakes. The group managers have been proactive in identifying key emerging technical areas that could benefit from knowledgeable postdoctoral fellows and research associates, and they have successfully recruited top technical talent for these positions. The division has experienced a 10 percent increase in personnel within the last 2 years, indicative of its success in attracting funding for its programs. The NRC postdoctoral program has been astutely used to attract recent Ph.D. graduates possessing the scientific expertise needed to support leading-edge research areas. Experienced postdoctoral fellows working at the MSED have also been a significant resource for the addition of new permanent staff. The continuity of technical effort is challenged when key technical experts retire or move to other assignments, even though in most instances the losses are foreseeable. This is particularly acute in areas that have fewer staff or that are highly dependent on research conducted by postdoctoral researchers. Usually, when the term of service of a postdoctoral researcher ends, there is either a short overlap or a technical talent gap, with resultant loss of continuity and technical knowledge on the project. A similar situation arises when a staff member retires. The consequences are an avoidable slowdown in the critical work of the organization.

For MML cross-cutting programs, there is no standard process to obtain input from industry, academia, and government laboratories (including government-owned, government-operated [GOGO] and government-owned, contractor-operated [GOCO] laboratories) on key program deliverables desired by users. However, all divisions, including the MSED, are strongly engaged with these organizations. Also, these cross-cutting programs currently have no standard means within the MSED to identify researchers in other divisions with suitable expertise who could contribute to the program. Because of the depth of the scientific talent within the division, the leadership and staff have been resourceful in establishing new programs at the request of industry and have been participating in cross-cutting initiatives. Researchers are highly committed to project success and engaged with high enthusiasm in their technical work. They mentioned several positive factors, which included working on important national and industrial problems; collaborating with other experts across the NIST campus; having freedom to conduct research in emerging areas and to address novel approaches for solutions to problems; the enterprise's commitment to develop comprehensive plans for long-term projects; and the strong connectivity they enjoy with external researchers at universities and other laboratories (government and industry) in selected areas of research and technology.

ADEQUACY OF FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

Facilities within each group in the division range from exceptional to adequate with respect to supporting the division's goals. The researchers also take advantage of equipment at facilities outside NIST when the cost and projected usage rate of such instruments indicates that it would not be cost-effective for NIST to purchase it. An example of the benefits that first-rate equipment offers is the exciting progress made in dimensional metrology by the Functional Polymers Group using the CD-SAXS with its application to lithographic patterning (particularly line edge roughness, sidewall geometry, and pattern fidelity). This is a very useful pattern characterization tool that has attracted substantial academic and industrial interest and support. With a synchrotron source, data acquisition takes only tens of seconds. With a common laboratory source, data acquisition takes tens of hours, which obviously hampers the utility and industrial adoption of the technique. The sensitivity of the analysis can be further improved using soft x-ray resonance enhancement (resCD-SAXS). Another example is the cruciform biaxial stress/strain testers with in situ optical and x-ray monitoring used by the Mechanical Performance Group. This unique piece of equipment can perform mechanical testing on a wide range of structural materials, providing critical data required by automotive design engineers using sophisticated computation tools; it will shorten the lead time to design lighter-weight vehicles. Also, NIST's scattering and reflectivity facilities and capabilities are excellent and provide capability for soft material analysis of both solids and solutions. nSoft provides a rapid proof-of-concept neutron scattering and reflectivity facility whose use does not require a detailed proposal or submission through the general user proposal process.

Maintaining and adding to the suite of cutting-edge facilities and equipment is a substantial challenge, subject to the perturbations of the NIST budget and financial policies. In pursuing new areas, or new directions, equipment acquisition becomes a pacing item. Because of bureaucracy and budget restraints, many instruments are largely home-built. While this often leads to specialization for a particular task, it also engenders a dependency on the creator of the software and hardware, which then becomes an issue when people leave.

Integrating the metallurgy expertise with polymer disciplines has been challenging and is a work in progress. The groups historically have not interacted much, but they are committed to identifying additional areas where they can leverage the knowledge and expertise of each discipline to provide fresh insight for tackling problems.

There has been a systematic erosion over many years of important technical support services, such as machine shop, print shop, glassblowing, and electronics support. This affects the efficient utilization of scientific talent. The ratio of scientific staff and postdoctoral researchers to technicians is very high. The availability of more technicians would free the scientific staff for more productive work.

In summary, the division has developed an excellent set of programs addressed by competent staff. The facilities acquired by the division are of high quality and are adequate to perform the current array of projects. The division faces resource challenges in areas that constitute avenues for further improvement.

DISSEMINATION OF OUTPUTS

Within NIST, the quarterly MML all-hands meetings and the quarterly MSED newsletter have been excellent means of communicating to the employees, many of whom are so immersed in their activities that they do not stay up to date on what else is going on. This communication is an important means of collaboration.

Every MSED activity has a specific plan for disseminating results, which may include attendance at workshops, presentations at technical society meetings and workshops, laboratory focus groups, NIST-sponsored workshops, demonstrations at NIST and partner facilities, publications, patents, and industrial visits. The formation of consortia, such as nSoft, has been a particularly effective dissemination method to industrial research organizations.

Since 2012, the division scientists have authored 173 papers in archival journals, produced 41 conference proceedings, led 13 workshops, co-organized 3 workshops, authored 8 NIST reports, concluded 3 material transfer agreements, and participated in 2 industry roadmapping committees and 45 standards committees. A total of 700 standard reference materials were sold or verified, and 6 invention disclosures were filed.

Staff reported that by policy, many junior researchers may attend only a single technical meeting a year, although they would build their knowledge and their networking with colleagues at universities, government laboratories, and industry—including collaborators at leading institutions—by attending meetings that are most relevant to their work, even if that means more than one meeting a year. While the usual criteria for selection (e.g., participating as organizer, plenary lecturer, or invited speaker) are clear and well known, attendance could be useful even when an attendee is not making seminal contributions. For example, attendance would enhance a researcher's knowledge of relevant and new research areas or improve their understanding of industry needs. These opportunities are valuable for the professional growth of the individual and, therefore, for NIST. The division needs to continue its aggressive customer outreach efforts, especially by seeking input from customers on which MSED outputs would be most valuable. This information would be quite useful in keeping the strategic plan up to date.

Within the research groups, there is a substantial focus on customer outreach, not only to disseminate the results of the research, but also to determine which MSED outputs would be most valuable to industry. This effort could be expanded as new projects are started.

OVERALL ASSESSMENT

The division has developed an excellent array of programs addressed by competent staff. The scope of efforts within the division is impressive, ranging in length scales from nanometers to meters. The types of materials and processes used in the investigations cover the gamut of advanced materials, from high-temperature superalloys to magnesium sheet, to sophisticated polymers, polymer composites, electronic and photonic materials, and multifunctional materials. The staff and facilities acquired by the division are of high quality and are adequate to perform the projects. NIST fellows, technical staff, postdoctoral researchers, and guest researchers are attracted by the culture of doing work important to the nation and by the opportunities to employ cutting-edge methods to accomplish their projects. The active involvement of division scientists in technical meetings and forums and their creativity in developing one-of-a-kind instruments are additional factors that keep the division at the cutting edge.

The recent reorganization of the division has increased collaboration opportunities among the different MSED technical groups, such as determining mechanical properties under extreme conditions and high-strain-rate loading conditions for polymeric and metallic materials. The cross-cutting projects, such as the Materials Genome Initiative and the additive manufacturing program, and the MML focus groups offer additional opportunities for collaboration among the technical disciplines. The division has many notable examples of external collaborations and customer outreach activities.

The development of a strategic plan and the formation of the Office of Data and Informatics are important works in progress. The newly initiated effort to develop an overall strategic plan for the MML will help in the identification and assessment of additional opportunities for research within the MSED and will provide a rational basis for balancing the resources and efforts across the groups.

The division has developed a portfolio of projects that encompasses an impressive array of technology challenges of importance to U.S. industry. The projects have brought to bear innovations and applications of measurement science that are crucial to advancing medicine, organic and semiconductor electronics, photonics, aerospace, automotive, and other scientific and technical areas useful to the industrial sectors. The division leadership and staff are making notable efforts in critical areas through an effective integration of technical expertise and facilities to address workspace challenges, including long acquisition time lines and onerous bureaucratic workloads associated with acquisition of equipment, services, and supplies.

FINDINGS AND RECOMMENDATIONS

The MSED materials informatics work supporting the Materials Genome Initiative is a challenging, ambitious effort within the national MGI effort. To be successful, the MSED will require multiple years of consistent and deliberate effort to identify gaps, develop experimental and theoretical program plans, and complete projects that are useful to the NIST users as well as external customers. However, until a detailed project roadmap has been constructed and validated, it will be challenging for the program to request additional funding. The newly established MML Office of Data and Informatics could be a significant asset to the NIST MGI effort.

Recommendation: The Materials Science and Engineering Division should develop a program roadmap for its Materials Genome Initiative (MGI) effort, detailing specific projects that will produce in the short term and the long term, identifying deliverables useful to the stakeholders, and specifying areas of Material Measurement Laboratory

strengths, opportunities, resource requirements, and priorities. The Materials Science and Engineering Division should develop and implement a systematic plan to obtain stakeholder input on the deliverables for the Materials Science and Engineering Division elements of the MGI program.

MSED's technical program director is responsible for identifying experts who can contribute to MGI and who coordinate and link cross-cutting tasks, although the standard method for identifying relevant NIST technical experts who can contribute to cross-cutting efforts was not explained.

Recommendation: For cross-cutting programs, the Materials Science and Engineering Division should establish a standard method to identify relevant NIST technical experts who can support its cross-cutting efforts.

MSED staff reported that there are ponderous institutional rules and procedures imposed at the enterprise level that need to be followed to acquire items ranging from needed routine items to major pieces of equipment, and that these are impediments that adversely affect the morale of the researchers and detract from the time that they can focus on their technical efforts.

Recommendation: The Materials Science and Engineering Division should work with Material Measurement Laboratory management and NIST administrative and legal offices to identify compliant ways to streamline the current rules and procedures for acquisition of equipment and support services.

The continuity of technical effort is challenged when key technical experts retire or move on to other assignments, even though in most instances the losses are foreseeable.

Recommendation: The Materials Science and Engineering Division should establish a yearly planning effort and succession plan to address the continuity of critical technical disciplines across the division.

DFT computational techniques are useful for one-dimensional structures (e.g., graphenes and nanotubes). Their utility for 3-D structures is more limited and requires integration with other computational tools. Their application for specific problems in the nanometer scale is worthwhile as is emphasis on phase equilibria, solid state, transformations, and kinetics. While DFT techniques can be very useful, this group appears overly focused on the technique and needs to expand its repertoire of techniques. The work presented was long on rationalization and short on prediction of properties for new structures and compositions and on matching material properties with new structures. This is not surprising for an early effort, but a balance between rationalization and prediction is necessary.

Recommendation: The Thermodynamics and Kinetics Group should develop an understanding of the limitations of density functional theory and should investigate and apply other tools in three-dimensional modeling for metals and soft materials.

Although the Thermodynamics and Kinetics Group provides considerable capability in computation and modeling, it is heavily focused on metals, alloys, and metallic structures. Other materials, such as amorphous solids, glassy materials, and polymers, are given less attention. These types of material are treated computationally in the Polymers and Complex Fluid Group, which studies molecular dynamics and coarse grain methods for polymers.

Recommendation: The Thermodynamics and Kinetics Group and the Polymers and Complex Fluid Group should better connect their computation and modeling efforts to

provide a more inclusive platform for computation and modeling and to foster a materials-by-design concept supporting the Materials Genome Initiative effort.

Development of magnetic nanoparticles for in vivo medical applications is of great biomedical importance, and it is being aggressively addressed by other research groups.

Recommendation: The Functional Nanostructured Materials Group should develop a strong link to medical community users of nanoparticles for in vivo medical applications and should reevaluate the direction and value of its contributions in light of the many efforts ongoing in the area.

From a research point of view, development of 3-D photovoltaics is a challenging proposition with significant external research underway.

Recommendation: The Functional Nanostructured Materials Group should evaluate related work worldwide and should concentrate its efforts on magnetic materials, energy storage, and nanowires to build on current successes, such as leveraging results on the lithium-ion battery.

Although the Polymer and Complex Fluids Group listed expertise in organic synthesis, an effort in organic synthesis was not evident in the presentations to the panel. The lack of synthetic expertise in both this group and the Functional Polymers Group could be viewed as an area in need of significant improvement, because without synthesis capability there is a highly limiting dependence on commercial materials or those generated through external collaboration.

Recommendation: The Polymers and Complex Fluids Group should consider establishing strength in polymer synthesis to support the measurements efforts, so that the researchers have ready access to state-of-the-art materials.

Membrane separation is a very important area, but many of the problems being addressed by the Functional Polymers Group are already being extensively investigated by others.

Recommendation: The Functional Polymers Group should evaluate related work worldwide on membrane separation and should consider redirecting its efforts toward unique scientific contributions that it could make in the many areas of industrial separations utilizing membranes.

The Mechanical Performance Group is heavily focused on metallic materials, a legacy of the previous organizational structure. There is a lack of emphasis on ceramic and ceramic composites, even those these are becoming important commercial material systems.

Recommendation: The Mechanical Performance Group should continue to integrate itself more closely with the groups working on soft materials and should consider the contributions that it could make to the testing of ceramic materials, such as ceramic matrix composites at high temperatures.

8

Key Findings and Recommendations

The creation of the Material Measurement Laboratory (MML) has yielded positive results. The discipline-specific projects for producing standards for traditional industries are evolving into flexible, collaborative, cross-disciplinary endeavors that are much more appropriate for addressing the needs of modern industry. Teams are formed within and across MML divisions that are capable of developing technology and standards for the characterization of advanced materials, such as biological therapeutics, nanomaterials, and organic electronics. Standards for such products will not only promote innovation and expedite development of manufacturing processes but will also facilitate evaluation and quality control for commercialization and interaction with regulatory organizations. The knowledge, technology, reference standards, and data developed by MML teams will contribute to quality assurance tools for addressing problems of national importance such as climate change, renewable energy, health care, infrastructure, food safety and nutrition, forensics, and homeland security.

Two factors have had the most impact on the evolution of the MML: (1) the collocation of staff members doing research into measurement systems and staff focused on characterization, production, and dissemination of standard reference materials and data and (2) mandated initiatives that are conducted by staff from many departments. The collocation of research and production staff has led to some confusion about the relative value of the different endeavors. However, the research staff are more focused on potential opportunities for new standards and measurement methods than they may have been earlier, while the individuals focused on production of reference materials are exposed to a broader spectrum of possible uses and opportunities for new standards. Both types of staff members take pride in their work, and senior management recognizes the value of both endeavors. More communication, more strategic staffing, and better personnel management training could facilitate sustainability of these interactions and the respective functions.

The mandated projects are demanded as a result of national initiatives, and MML management and staff want to address these important problems. In some cases, such as forensics, preexisting projects are reoriented to address the mandates to the extent possible. For additive manufacturing or safety of nanomaterials, MML management, staff, and external stakeholders do a very good job of defining a program that spans divisions to take advantage of relevant expertise and facilities and specifying potential objectives that will make a critical difference to the initiative in terms of measurement capabilities, reference materials and data, and technology transfer. Based on reports by MML staff, one area where these cross-cutting programs could improve is communicating the measures for success to staff members doing the work in the various divisions, so that each individual can understand how their part fits into the whole or what balance of their effort is appropriate for different projects. According to comments from the MML staff, most of the technical expertise required to support the cross-cutting initiatives is available within the MML or the broader NIST community, although identifying appropriate participants may be difficult. If the biobased initiatives are expanded, additional staff may be required in relevant areas, because these biologically oriented disciplines have not been pursued to such a significant extent at NIST. The expansion of the informatics operation (at Office of Data and Informatics, ODI) is essential because the MML needs increasingly to evaluate complex data sets and extract meaningful knowledge for assessing the validity and relevance of the measurements and extracting knowledge.

In general, the quality of the research programs is comparable to that at other premier research institutions. While interesting scientific observations are valued, the work is very much targeted at the production of new measurement methods, data, and standards of use in knowledge generation and manufacturing. The staff publishes in refereed journals at a reasonable rate, with occasional papers published in tier 1 journals, but most of the publications are more archival in nature and can be found in specialty journals where they will reach an application-specific audience. The patent process is not well developed at NIST, and this is problematic for the development of intellectual property, which might be useful for expanding the scope of the MML mission by encouraging commercialization of MML-developed measurement technologies and production of standard reference materials.

As the focus of MML activities evolves and the need for new types of standards and reference materials becomes clear, there is a concern that the areas in which the MML has previously excelled may be lost. For example, NIST has an international reputation for characterization of ceramics and for mass spectrometry of chemicals. Such expertise needs to be maintained as the expansion into biomaterials and nanomaterials receives increased attention.

The MML is very well supported in terms of facilities and equipment, but MML staff reported that administrative support at the NIST level for purchasing, contracts, and legal review slow technical progress. The equipment provided to support the technical programs is generally state-of-the-art. However, the new overhead structure decreases funds available for equipment, and the maintenance costs are considerable. The overhead structure was changed to encourage the devotion of more resources to manpower. This is not necessarily a bad policy, but the MML will be less able to purchase one-of-a-kind items like the Brookhaven beamline or the 900 MHz nuclear magnetic resonance (NMR) machine. The allocation of space needs to be reevaluated from the standpoint of laboratory functionality in order to optimize efficiency and reduce clutter from outdated or unused equipment. Purchasing procedures, contracts management, and legal review are not timely, even compared to other government laboratories. Such operations should be reviewed independently and streamlined as much as possible to help accomplish the NIST mission.

The MML works hard to involve its stakeholders at all levels, by establishing programmatic priorities, collaborating on individual projects, and providing feedback on the utility of reference materials. Topic-specific workshops seem to work particularly well. Communication with stakeholders is an ongoing challenge that demands constant attention. The establishment of project leaders who coordinate outside queries and interests with internal experts has been a useful tactic that should be expanded. Creating and maintaining a more informative website would also be helpful. The MML is cognizant that interactions with potential industrial, government, and academic beneficiaries of their programs is critical to making the right choices in project directions and utilizing the technologies and reference materials developed, and MML staff are constantly exploring new approaches to encourage interactions. In addition to the sales of reference materials, information is distributed to the public by other means such as dissemination of web-based data sets, inclusion of data with commercial instruments (e.g., mass spectrometry library), and publications, and the success of these methods is monitored with the goal of ongoing improvement. Licensing technology has not been a significant mechanism for technology transfer; this is an opportunity wasted. More support for modern web-based communications, faster approvals for collaborations and materials exchanges with industry and other government agencies, and more flexible travel policies would all improve the sharing of MML expertise with stakeholders.

Traditional endeavors at NIST prior to the formation of the MML focused on research to improve measurements and development of standard reference materials and data. The work was performed by small groups in divisions stovepiped by academic area. This type of traditional endeavor continues, but now MML scientists and engineers are expected to interact across disciplinary boundaries and participate in large-scale initiatives that require interdisciplinary collaboration within NIST and across the nation. The research-oriented staff generally find this change exciting and enabling, but staff whose primary function has been supporting production of standard reference materials are, in many cases, unclear about their value in the new organization. The general caliber of technical expertise is competitive with the best large research institutions in the country, but the products generated are generally more varied, because standard reference data, materials, and methods are just as important at the MML as seminal publications or patents.

The findings and recommendations below focus primarily on opportunities to increase the productivity of the MML as a highly valuable and targeted national resource with the potential to play an even greater role in U.S. innovation and competitiveness and to provide an even more broadly based inventory of metrics for use by industry and regulatory agencies.

The MML continues outstanding technical performance in areas related to NIST's traditional endeavors—that is, producing reference materials and supporting the development of international standards. In some cases, the groups in the MML have reached their capacity to support production of reference materials. It is critical for national innovation and industrial competitiveness that leadership in standards development and production of reference materials be supported by first-rate staff and state-of-the-art equipment.

Recommendation 1. The Material Measurement Laboratory should develop a strategy, with significant input from stakeholders, especially industry, to determine which standard reference materials (SRMs) should be terminated, continued, or added. Succession planning for technical staff and project leadership should be carefully addressed to make sure that the capabilities and corporate knowledge pertaining to SRMs do not erode over time. Total manpower and the balance between technicians and Ph.D. staff, financial allocations, pursuit of intellectual property to induce industrial production of SRMs, and other aspects of the process of standards production should be included in the strategic evaluation.

The MML is developing reference data and materials to support industries that are not as well established, including standards for biological materials, nanomaterials, and advanced materials-based products. MML staff are working hard to establish and maintain relationships with relevant industrial and regulatory stakeholders. The identification of which standards or measurement technologies will expedite the critical paths for processing and validation is very difficult. The role of area-specific project coordinators to funnel external queries to the appropriate NIST expert is proving extremely useful. Personnel exchanges with industry would be very useful: MML staff would better understand the development-to-product process and industrial partners could provide input for standards selection. For example, industry fellows could spend time at the MML, and MML staff could spend short sabbaticals learning industrial production processes.

Recommendation 2. The Material Measurement Laboratory (MML) should make much more apparent the focal points for channeling external interactions. The MML should increase the number of project coordinators to funnel external queries to the appropriate NIST expert. The MML should ensure that its portion of the NIST website is updated to market MML capabilities and activities more effectively to potential users of standard methods and materials. The MML should develop additional mechanisms to increase its interactions with industry.

The MML is starting new research initiatives and programs to be responsive to national mandates. These initiatives bring researchers together across MML divisions, across NIST, and externally, with the result that MML staff are very aware of needs and trends for the future. The MML has named technical program directors to manage cross-cutting initiatives across division boundaries. However, at the group level, the near-term objectives and expected deliverables are unevenly defined and the quality of the research is highly variable.

Recommendation 3. The Material Measurement Laboratory should perform technical assessments of research projects at the group, division, and laboratory levels to evaluate the balance between productive existing efforts and new initiatives, to ensure a balance that

supports the Material Measurement Laboratory mission, is consistent with available resources, and clearly states the objectives and expected products to all participants.

The ODI has recently been established, and its director has been hired. The ODI will play an important role in support of the Materials Genome Initiative (MGI). However, other MML projects and initiatives are producing highly complex data and need to extract meaningful information from that data. Resources capable of manipulating complex data, data mining to produce knowledge, and disseminating the findings are needed across the MML. The reorganization of the MML has provided opportunities for increased collaborations. One example of leveraging external collaboration is the placement of MML staff at Stanford University to develop biological measurement science, where interactions with faculty and students is a win-win experience for both MML and Stanford.

Recommendation 4. The Material Measurement Laboratory (MML) should provide the resources required by the Office of Data and Informatics (ODI) as rapidly as possible. The MML should integrate the ODI into activities across the MML, especially with any divisions producing information on biological/organic systems. To the extent possible, the MML should leverage outside collaborations while building its own capacity; it should consider using the satellite facility at Stanford as a beachhead to strengthen such connections.

The staff are empowered by the continuity of funding. They are enthusiastic about the opportunity to contribute to national innovation and competitiveness by producing better measurement methods and standards. Staff reported that productivity is clearly hampered by slow responses and multiple levels of administrative oversight external to the MML, especially in the areas of contracting for purchases of supplies and equipment and for legal approvals for industry interactions, work for other government agencies, and use of clinical materials. Achieving the mission of the MML suffers when the controlling priority is compliance with legal and contracting procedural stipulations; both mission accomplishment and compliance should be possible if the priorities are rationally balanced.

Recommendation 5. The mission priorities of Material Measurement Laboratory (MML) scientists and NIST administrative and legal staffs should be aligned. The MML should work to ensure that (a) its staff scientists have simplified training in contracting procedures so they can provide the necessary information at the beginning of a procurement process, and so contracting staff can see how they help the MML to achieve its technical mission; (b) unnecessary legal review and rereview is curtailed by bringing the processes into compliance with standards in other government laboratories and by delegating approval authority; and (c) standard times for review are established to manage MML staff expectations and planning.

The recent reorganization of NIST and the MML has brought the research and standards efforts into much closer contact, in many cases resulting in staff members participating in both endeavors. Therefore, the research is more clearly targeted at producing better measurement systems that will facilitate manufacturing and quality control. Nonetheless, the melding of the standards and research cultures is not without challenges. Some MML staff expressed concerns about the management's perceptions of relative values of traditional activities versus newer research and development activities. Personnel management is uneven. The demonstration project process for personnel evaluation is generally good but needs to be improved. It is administered in different ways in different divisions, and an unacceptable number of supervisors are perceived by staff as ineffective in motivating staff or fostering career development.

Recommendation 6. The Material Measurement Laboratory (MML) should ensure that at the project level the objectives and interrelationship between research and standards

development are clearly stated and that supervisors at all levels make clear that both research and standards products/metrics are considered important elements of personnel evaluation, resource allocation, and intellectual regard. The MML should enhance understanding of the performance expectations by providing to all staff annual tutorials covering expectations and metrics for productivity and impact. The MML should establish clear and uniform approaches for creating individual performance plans and reviews; should ensure that reviews are administered using the same process; and should provide supervisor training for all supervisors who have not already taken such training.

Acronyms

2-D LC-MS	two-dimensional liquid chromatography-mass spectrometry
ACMD	Applied Chemicals and Materials Division
ADA	American Dental Association
AFM	atomic force microscopy
ALD	atomic layer deposition
ANSI	American National Standards Institute
ASTM	American Society for Testing and Materials
BBD	Biosystems and Biomaterials Division
BCARS	broadband coherent anti-Stokes Raman scattering
BMD	Biomolecular Measurement Division
BMM	beam line for master measurements
BSA	bovine serum albumin
CD-SAXS	critical dimension measurement by small-angle x-ray scattering
CD-SAXS	critical dimension small-angle x-ray scattering
CHO	Chinese Hamster Ovary
CMOS	complementary metal-oxide-semiconductor
CNTs	carbon nanotubes
CRADA	cooperative research and development agreement
CRP	C-reactive proteins
CSD	Chemical Sciences Division
DARPA	Defense Advanced Research Projects Agency
DATA	Digital Accountability and Transparency Act
DFT	density functional theory
DHS	Department of Homeland Security
DNAA	delayed neutron activation analysis
DoD	Department of Defense
DSQAP	Dietary Supplement Laboratory Quality Assurance Program
EPA	Environmental Protection Agency
ERCC	External RNA Controls Consortium
ES-DMA	electrospray-differential mobility analysis
FARS	frequency-agile, rapid scanning spectroscopy
FDA	Food and Drug Administration
FIB	focused ion beam
FRET	fluorescence resonance energy transfer
GOCO	government-owned, contractor-operated

GOGO	government-owned, government-operated
HAXPES	hard x-ray photoelectron spectroscopy
HER2	human epidermal growth factor receptor 2
HITRAN	high-resolution transmission
HPCVD	handheld point chemical vapor detector
IBBR	Institute for Bioscience and Biological Research
ICP-MS	inductively coupled plasma mass spectrometry
IIS	Innovation and Industry Services
INAA	instrumental neutron activation analysis
IP	intellectual property
IS	institutional services
ISI	Institute for Scientific Information
ISO	International Organization for Standardization
LC–MS	liquid chromatography–mass spectrometry
MGI	Materials Genome Initiative
miRNA	microRNA
MML	Material Measurement Laboratory
MMSD	Materials Measurement Science Division
MRD	Materials Reliability Division
MSED	Materials Science and Engineering Division
NanoEHS	nanotechnology environment, health, and safety
NCI	National Cancer Institute
NEXAFS	near-edge x-ray absorption fine structure
NIH	National Institutes of Health
Ni-MH	nickel–metal hydride
NIST	National Institute of Standards and Technology
NRC	National Research Council
NSLS	National Synchrotron Light Source
NTRM	NIST Traceable Reference Material
ODI	Office of Data and Informatics
OLED	organic light-emitting diode
ORM	Office for Reference Materials
PGNAA	prompt gamma neutron activation analysis
PMA	Pharmaceutical Manufacturers' Association
POP	persistent organic pollutant
qNMR	quantitative nuclear magnetic resonance
qPCR	quantitation using the polymerase chain reaction
REFPROP	Reference Fluid Thermodynamic and Transport Properties Database
RNAA	radiochemical neutron activation analysis
SAM	self-assembled monolayer
SEM	scanning electron microscope

SIMS	secondary ion mass spectrometry
SMG	Structural Materials Group
SPARC	stratosphere–troposphere processes and their role in climate
spICP-MS	single-particle, inductively coupled analysis plasma-mass spectrometer
SRD	standard reference database
SRM	standard reference material
STR	short tandem repeat
STRS	scientific and technical research and services
TGA	thermogravimetric analyses
TOFMS	time-of-flight mass spectrometry
TPD	Thermophysical Properties Division
TRC	Thermodynamics Research Center
USDA	U.S. Department of Agriculture
UV-Vis-NIR	ultraviolet, visible, and near infrared
WMO	World Meteorological Organization
WMO-GAW	WMO global atmosphere watch
XAFS	x-ray absorption fine-structure spectroscopy
XPS	x-ray photoelectron spectroscopy