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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:

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Summary

The Chemical Science and Technology Laboratory (CSTL) is meeting its obligations, and its priorities are appropriate and aligned with national priorities. The technical merit of the laboratory and the commitment of the staff are high. There is no evidence that any programs are jeopardized by a lack of facilities or equipment. Future assessments will be facilitated if greater emphasis is placed on clarifying the distinctions between work performed to provide services and work performed to support research and development. Against this backdrop of clear and consistent success and high technical merit, the panel has the following comments about the operation of the Laboratory:

1. The set of criteria known as “5+1” for ensuring that the research projects are aligned with the mission of NIST and the laboratory should continue to be used. The CSTL leadership should link its more basic research investments to the potentially important measurement-related outcomes that are envisioned to result from CSTL research.
2. The CSTL leadership should put more effort into communicating to the staff the rationale for resource allocation between new initiatives and established programs, some of which produce revenues through standard reference materials (SRMs). One example is the current focus on nanoscience and nanotechnology, which competes with established metrology.
3. CSTL should continue its practice of cross-pollinating research planning teams with individuals from different divisions as new initiatives are developed.
4. There is a sense that a greater fraction of research is being directed at computation than at experimentation and instrument development. The CSTL leadership should examine this trend to assess its impact on future capabilities of the laboratory.
5. CSTL should consider special efforts, such as interdivisional seminars and study groups, to generate more interest in interdisciplinary projects and to avoid redundancy in research projects across divisions.
6. The CSTL leadership should carry out its planned efforts to communicate to the staff the incentives for disclosing intellectual property and applying for patents.
7. The ratio of Ph.D. scientists to technical and office support staff appears to be so high that the Ph.D. scientists are often required to perform a technician’s work to accomplish a task. Besides serving as a barrier to the recruitment of outstanding scientists, this imbalance reduces the research productivity of the scientists. CSTL leadership should assess the ratio of support staff to Ph.D. scientists in terms of its effect on recruitment and productivity.
8. It is not clear that the laboratory has developed guidelines for replacing scientists in critical areas who retire or leave the laboratory for other reasons.

The laboratory should develop a strategic plan to address recruitment issues and identify areas of opportunity and areas of concern.

9. The CSTL should increase efforts to make its scientists more visible in their respective scientific communities.

Charge to the Panel and Description of the Assessment Process

At the request of the National Institute of Standards and Technology (NIST), the National Academies, through its National Research Council (NRC), 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 eight,[1] as well as the adequacy of the laboratories' resources. In 2007 NIST requested that four of its laboratories be assessed: the Chemical Science and Technology Laboratory (CSTL), the Electronics and Electrical Engineering Laboratory, the Information Technology Laboratory, and the NIST Center for Neutron Research. Each laboratory was assessed by a separate panel of experts, and the findings of each panel are summarized in separate reports. This report summarizes the findings of the Panel on Chemical Science and Technology.

NIST requested that the panel consider the following criteria as part of its assessment:

1. The degree to which the Laboratory programs in measurement science, standards, and technology address national priorities.
2. The degree to which the Laboratory programs in measurement science, standards, and technology are well-motivated with regard to the following questions:
   a. What is the program trying to accomplish?
   b. What is innovative or different, as compared to efforts at other institutions, about the program's approach that will lead to success?
   c. Is success well defined?
   d. What will be the impact of success?
   e. How will success be disseminated to end users?
   f. How much will success cost, and how long will it take?
   o The technical merit of the Laboratory programs relative to the current state of the art worldwide.
3. Insofar as they affect the quality of the technical programs, the adequacy of the Laboratories' facilities, equipment, and human resources.

To accomplish the assessment, the NRC appointed a panel of 19 volunteers whose expertise matched that of the work performed by CSTL staff. The panel members were also assigned to five subgroups whose expertise matched that of the work performed in the five divisions in CSTL: Analytical Chemistry, Biochemical Science, Physical and Chemical Properties, Process Measurements, and Surface and Microanalysis Science. These subgroups of the panel separately visited CSTL facilities for 1 or 2 days, during

[1]The eight NIST laboratories are the Building and Fire Research Laboratory, the Chemical Science and Technology Laboratory, the Electronics and Electrical Engineering Laboratory, the Information Technology Laboratory, the Manufacturing Engineering Laboratory, the Materials Science and Engineering Laboratory, the NIST Center for Neutron Research, and the Physics Laboratory.

which they attended presentations, tours, demonstrations, and interactive sessions with CSTL staff. Subsequently, the entire panel assembled for 1.5 days, during which they attended overview presentations by CSTL management and interactive sessions with CSTL managers; the panel also met at this time in a closed session to deliberate its findings and to define the contents of this assessment report.

The panel's approach to the assessment relied upon the experience, technical knowledge, and expertise of its members, whose backgrounds were carefully matched to the technical areas within which the CSTL activities are conducted. The panel reviewed selected examples of the standards and measurements activities and the technological research presented by the CSTL; it was not possible to review the CSTL programs and projects exhaustively. The panel's goal was to identify and report salient examples of accomplishments and opportunities for further improvement with respect to the technical merit of the CSTL work, its perceived relevance to NIST's definition of its mission in support of national priorities, and apparent specific elements of the CSTL's resource infrastructure that is intended to support the technical work. These highlighted examples, for each CSTL division, are intended to collectively portray an overall impression of the laboratory while preserving useful mention of suggestions specific to projects and programs that the panel considered to be of special note within the set of those examined. The assessment is currently scheduled to be repeated biennially; while the panel applied a largely qualitative rather than quantitative approach to the assessment, it is possible that future assessments will be informed by further consideration of various analytical methods that can be applied.

The following report sections provide an assessment of each of the CSTL divisions and are organized into four areas:

- The degree to which CSTL programs in measurements and science and standards address national and agency priorities;
- The impact and innovativeness of the programs;
- The technical merit of the CSTL programs relative to the current state of the art worldwide; and
- The adequacy of the facilities, equipment, and human resources that affect the quality of the CSTL's technical programs.

More detailed information on CSTL activities and programs can be found on its Web site: www.cstl.nist.gov/ or its published documents. CSTL's Web site in particular highlights programs, projects, and technical activities at the Laboratory, lists publications, and provides information on its products and services and other developments.

Analytical Chemistry Division

SUMMARY

The Analytical Chemistry Division (ACD) has been meeting its obligations, and its priorities are appropriate. The technical merit of the division, the commitment of the staff, and availability of equipment and facilities are of a high order. Future assessments will be facilitated if the ACD presentations to the NRC panel place greater emphasis on separating service activities from development and research activities and if the status of and progress on projects are clearly reported.

ADDRESSING NATIONAL PRIORITIES

The ACD is involved in new NIST-level programs on standards and methods to address the challenges of the hydrogen economy, climate change, nanotechnology, biofuels, and medical diagnosis. These challenges provide a framework for development of improved metrical methods, standards, and materials. The issues involved in new and renewable energy, environmental stewardship and measurement accuracy, and improvements in health and medical research are important national priorities.

The Inorganic Chemical Metrology Group is addressing biology as metal-protein complexes (metallomics); the biogeochemical cycling of sulfur and the formation of sulfate (SO_4^{2-}) aerosol particles in the atmosphere; the oxidation states of arsenic; organometallic species in marine tissue standard reference materials (SRMs); sulfur at levels of less than a microgram per gram in diesel and gasoline SRMs; and the measurement of small quantities of fissionable nuclides such as ^{235}U and ^{239}Pu. Such projects are in response to requests from outside agencies as well as industrial consortia.

The mission of the Organic Chemical Metrology Group includes the development, critical evaluation, and application of methods for the identification and measurement of organic and organometallic species using analytical separation techniques and mass spectrometry. This mission is addressed by the measurement of organic compounds in support of the development of SRMs, quality assurance programs, and other agency activities in clinical, food and nutritional, environmental, forensic, and homeland security areas. This work is in alignment with essential national priorities. The addition of work that addresses nanotechnology would also be aligned with national priorities.

The Gas Metrology Group has focused on dynamic dilution for reducing uncertainties in gas standards; global climate studies; a volatile organic compound standard for environmental and hazard monitoring; the development of reference materials based on input from organizations such as the AIGER (Automobile Industry/Government Emissions Research) consortium; and the development of standards and methods to determine and monitor the concentration of ozone in the atmosphere. These projects reflect input from industry and industrial consortia that need high standards for purity and effective methods related to gas and emissions monitoring. The group must prepare itself to play a critical metrology role in any carbon emissions trading system that may be implemented to address global climate change.

For over two decades, the ACD has been involved in the banking of environmental specimens and analytical programs to ensure marine quality; these activities are collaborative efforts supported by NIST resources and funding from other federal agencies. The division currently maintains environmental specimen banks at two locations: the National Biomonitoring Specimen Bank at the NIST Center for Neutron Research in Gaithersburg, Maryland, and the Marine Environmental Specimen Bank at the Hollings Marine Laboratory (HML) in Charleston, South Carolina. The banks support important work in medicine and marine chemistry and biology.

NIST is the lead agency for metrology in nanotechnology. The accurate and comprehensive assessment of the risks to health and the environment posed by nanoparticles and nano devices is important. ACD staff typically develop methodologies by using and evaluating commercial instrumentation. This is a reasonable approach that gives their work direct impact across the ACD constituent communities. However, the ACD should be more involved in advancing technology to improve environmental monitoring, homeland security, forensic investigation, and clinical diagnosis. As the premiere analytical agency in the United States, it could play a more central role in developing new measurement techniques and in advancing the science of metrology into the biological and nanotechnology areas. Such fundamental studies will, however, require additional funding and should not be done at the expense of the ACD's current work on developing standards and methods.

IMPACT AND INNOVATION

ACD supports the mission of the CSTL by adhering to the vision it states as follows:

> To be recognized as the nation's reference laboratory for chemical measurements, providing traceability through measurement technology, reference materials, reference data, and other measurement services required to meet science and technology needs.

This vision is being realized through a strategy to conduct research on the qualitative and quantitative determination of chemical composition; develop and maintain state-of-the-art chemical analysis capabilities; disseminate tools for measurement traceability and quality assurance (such as reference materials, reference data, and other services); and demonstrate comparability of U.S. standards for chemical measurement with those of other national metrology institutes.

These core competencies allow the ACD to carry out its broad mission and give it the flexibility to respond to changing and evolving national priorities. In 2007 these competencies reside in three main groups: the Inorganic Chemical Metrology Group, the Organic Chemical Metrology Group, and the Gas Metrology Group. The organization was recently restructured to improve efficiencies and manage specific activities through multidisciplinary teams better able to address the changing landscape of analytical sciences.

The three primary groups collaborate in a number of high-priority program areas, including reference measurement methods and standards for environmental quality; clinical diagnostics; food, dietary supplements, and nutritional assessment; forensics and homeland security; commodities characterization; and advanced materials characterization.

Internationally recognized reference methods support the division's infrastructure for providing traceability for the chemical measurements used in programs of national and international importance through SRMs, NIST traceable reference materials, measurement quality assurance programs in critical areas, and comparisons of NIST chemical measurement capabilities and standards with those of other national metrology institutes.

The technical merit of scientists within ACD has been acknowledged in a number of different ways. During 2006, research in the division resulted in 60 peer-reviewed publications with an additional 28 manuscripts in press, down from an average of 106 publications per year over the preceding 4 years. In addition, staff gave 137 scientific technical talks, which is also fewer than the 196 talks in 2005. The status of the division with respect to other metrology communities at home and abroad is demonstrated by staff participation in 127 scientific committee assignments, up from 100 in 2005, and at the average of 128 over the preceding 4-year period.

In the area of fuel cell imaging technology, an exploratory research project has led to the conception and design of a new neutron-radiation-based imaging system that, when implemented, will allow the observation of the chemical actions in a fuel cell or across single biological cells. Applications such as biological cell imaging then become possible with this high resolution, as well as the ability to map the flow characteristics of hydrogen species across the proton exchange barrier of a hydrogen fuel cell. The development of SRMs for use in the biofuel industry should receive continued support, given the explosion of industrial activity in biofuels over the last year.

The electrochemistry activity is now down to one person. This calls into question the future viability of this program, and ACD must consider the intellectual losses that would result from the disappearance of this group.

In the area of nanoscience metrology, the collaboration with the National Cancer Institute and the Nanotechnology Characterization Laboratory (NCI/NCL) creates a natural link, especially given the topics—for example, gadolinium (Gd) and quantum dots. NIST is an ideal partner for NCI in this work. Gd and quantum dots have significant implications for many industries.

Projects at the HML continue to be relevant, effective, and impressive in quality. The work on contamination of waterways by flame retardants and on illicit and prescription drugs is worthwhile and appears to be progressing in a satisfactory manner.

Dietary supplements are an expanding field being explored by numerous agencies and governments. International collaboration is essential to prevent duplication of effort. The list of compounds being investigated by the division was proposed by the National Institutes of Health and the Food and Drug Administration. Given the wide diversity of both domestic and imported compounds and the multi-billion-dollar industry they support, this work could result in new mandated SRMs for controlling imports.

Work on the detection of trace explosives was very impressive. Given the current relevance and rapid growth of homeland security efforts, this and related work deserves even greater emphasis. To the extent possible, ACD should position itself as the leading metrology group for new methods of analysis applicable to homeland security.

In the area of proteomics and biomarker standards, health status markers have been identified as having high priority for immediate studies. Because protein biomarkers occur naturally with considerable heterogeneity (i.e., with glycosylation, acetylation, phosphorylation), the group has developed liquid chromatography and mass spectrometry techniques for chemical characterization of the target species, particularly the protein-based markers such as troponin I and prostate-specific antigen. This work is critical to continued biotechnology efforts.

TECHNICAL MERIT

Overall the technical merit of the division is excellent. Increased effort could be expended in developing analytical technology as well as methods and SRMs. Research in new technologies to advance the analytical sciences in any particular field seems to be left somewhat up to the individual group leaders and their views on how assertively to investigate such new measurement technologies. If the group leader exhibits leadership and is motivated to move an analytical technique forward, then that technique is included in the group's activities.

The technical merit of the Inorganic Chemical Metrology Group projects is, overall, very good to excellent. The emphasis on isotopic metrology for elemental isotopic measurements is highly appropriate. This is in many ways a breakthrough project leading to improvements in fundamental understanding of geological eras and origins of Earth and the planets. It enables improved understanding of biological processes such as kinetics and life cycles. The work on sulfur in diesel fuel is good, and the work on arsenic in drinking water is first rate and will result in additional reductions in detection limits and increased identification of specific arsenic species. The work associated with the various programs and projects in mass spectrometry, x-ray fluorescence, optical spectrometry, and sample preparation is proceeding well and underpins the productive role of this group in creating, developing, and maintaining the SRMs that constitute nearly three-fourths of ACD's products.

The Organic Chemical Metrology Group is developing standards and methods to determine the levels of specific proteins and other biomolecules in blood as indicators of certain disease states. This effort is largely motivated by proteomic biomarker discovery research supported in part by the NCI. There is currently enormous government and industry investment in developing protein biomarkers for specific disease states, and the results of this ACD group have shown a dramatic need for improved metrology. Needed to establish a quality assurance infrastructure for protein biomarker measurements are reference materials of known composition and stability; reference measurement procedures; and reference data libraries. Efforts are under way at ACD in each of these areas to establish measurement traceability and reliability. The group's research activities in separation science continue to investigate the physical and chemical processes that influence retention in liquid chromatography, gas chromatography, supercritical fluid chromatography, capillary electrophoresis, and capillary electrochromatography. Results from these fundamental studies are used to design stationary phases tailored to solve specific separation and analysis problems and to assist in method development and optimization. Additionally, during the past 2 years, the group has measured a number of SRMs of importance to the clinical, environmental, and food and nutritional communities.

The metrology sciences applied by the Gas Metrology Group are state of the art for this industry and have generally served as a benchmark for other domestic standards and gas measurements. The group has been conducting important projects in dynamic dilution, reference standards for the automotive industry, and ozone measurements.

The balance between services work and advanced technology or methods research is the key distinguishing characteristic of the programs of this division. The programs having a high service load relative to SRMs and international comparisons do not have the resources of time or personnel to pursue cutting-edge or proactive research. This disturbing aspect of the project planning process greatly reduces opportunities to perform the research necessary to address future—as opposed to present—customer needs. The scientific expertise within NIST is a national resource that should be valued highly. The scientists must have enough time to incorporate cutting-edge research into their portfolio. A number of programs have indeed been successful in obtaining extramural funds and are fulfilling the vision and mission of NIST—that is, meeting future challenges.

INFRASTRUCTURE

The division employs approximately 88 scientists, technicians, and administrative/clerical support staff. It has an annual budget of about $21 million, about $5 million of which supports programs of other federal and state government agencies and/or American industry on a cost-reimbursable basis.

The division recently experienced a reduction in full-time positions. Over the last 4 years there has been a steady decrease in personnel, specifically in the permanent lines. Eleven permanent professionals were lost from this division mostly owing to their transfer to the Biochemical Science Division. Reductions in scientific personnel have particularly profound consequences in this division because its SRM program and international activities result in a very high service load, and it is tasked with a leadership role in nanotechnology as well as support roles in homeland security, global climate change studies, and the new hydrogen economy. In particular, the Gas Metrology Group has been constrained in developing new gas measuring technologies and associated methods because it does not have enough Ph.D. staff.

Recent research in organic chemical metrology within the division has focused on techniques for characterization and quantitative determination of organic compounds, including proteins, in biological matrices. In FY05 and FY06, several new instruments were purchased that significantly increased the division's capabilities for the determination of trace-level analytes of health, nutritional, forensic, and environmental importance, as well as its ability to characterize proteins and other biomolecules and natural products.

The acquisition of an ultra-high-pressure, high-performance liquid chromatograph should be considered soon. This instrument is used routinely in the pharmaceutical industry to achieve improved separation efficiency and faster analysis. Maintaining state-of-the-art core competency requires this addition. New SRMs for both organic nanoparticles and atmospheric aerosols will likely be needed to support the fast growth of nanoscience and nanotechnology and the increasing interest in climate change. The addition of personnel with expertise in the mass spectrometry of environmental aerosols and the characterization of nanoparticles is recommended and is consistent with NIST's interests. ACD's interest in nanoparticle characterization logically overlaps with that of other NIST divisions.

Reconfiguration of the ACD has brought some improvement, particularly with the integration of the Nuclear Analytical Methods Group and the Inorganic Chemical Metrology Group and the transfer of the microfluidics activity to another division. Also the direct reporting of the HML specimen bank team to the Division Chief is a reasonable change that promotes efficiency.

Both the Gas Metrology Group and the electrochemistry program within the Inorganic Chemical Metrology Group are short-staffed by several positions, given current and potential future needs in these areas.

ACD has made commendable efforts to combat increased operating costs while still allowing for new projects to be mounted and existing projects to be continued. The increased charges for SRMs have alleviated some problems, and new funding by Congress is predicted to allow most activities to continue. In the face of increasing overheads, the division should critically assess the cost of maintaining such a large inventory of SRMs and determine the consequence of eliminating those in very low demand.

CONCLUSIONS

Additional Ph.D.-level staff should be recruited to prevent the loss of critical expertise and to allow the NIST knowledge pool to expand into critical areas such as proteomics, environmental aerosol mass spectrometry, and nanoparticle characterization. The potential loss of expertise in the following areas is of concern: gas metrology; electrochemistry; glass mixing, cutting, and polishing with the high precision required for SRMs; and precision machining for SRM quality fixtures. With the high skill levels required in the production quality of SRMs, neglect of these functions could seriously jeopardize future SRM quality or costs of production. These important support services are of vital interest to the entire CSTL.

ACD program design and planning are very good. The new cross-divisional planning exercise (addressing program opportunities in nanoscience metrology and in bioscience, including biomarkers and systems biology) conducted at the CSTL has had a positive impact on ACD and should also help ACD to integrate its work with other divisions within and outside CSTL. The mechanisms for determining project priorities and urgencies come from government directives and funding of projects as well as feedback from industry and committee interactions. ACD has not promoted its contributions and accomplishments at a level commensurate with the magnitude of its contributions to the field of analytical chemistry. The result of this underpublicized activity is that industry, academia, and other government laboratories may not be aware of some cutting-edge standards and methods and may be applying antiquated techniques for their own operations.

The laboratory should carefully consider the real costs of SRM development and recertifications for specialized industries where only a few SRM samples are purchased. ACD should reconsider its pricing for SRMs where high-profit industries are requesting only a few SRM samples. Indeed, its current SRM pricing structure does not reflect the cost of producing such standards and the supporting infrastructure required to maintain world leadership in standard materials. In such cases, it could impose a surcharge based on actual costs.

Specimen banking and marine quality assurance activities should be maintained. These banked specimens might one day be used to address issues of marine environmental quality and ecosystem changes through retrospective analyses and as such constitute a critical national resource.

Additional time and effort must be expended in mentoring and guiding the staff of other NMIs not having the skill sets and training of the ACD scientists. The participation of ACD staff in international comparison activities is vital to its own mission and function. Resource constraints could eventually begin to limit these necessary interactions. The constraints include time available to perform comparisons, generate reports, and travel; and staff shortfalls, especially in the Gas Metrology Group.

Efforts should be made to reduce the burdensome tasks of SRM maintenance, which is currently performed by the most highly qualified staff. The division should also help to make its scientists more visible in their respective scientific communities.

A strong molecular spectroscopy effort should be built within the ACD, because this capability was transferred to the Biochemical Science Division but is still needed within the ACD.

Biochemical Science Division

SUMMARY

The CSTL and new division leadership are making an impressive start in revitalizing this important area where NIST is expected to have strong growth. The Biochemical Science Division (BSD) has a wide array of scientific activities ongoing in three groups: DNA Measurements, Biospectroscopy, and Cell and Tissue Measurements. Structural biology at the Center for Advanced Research in Biology (CARB) and microfluidics activities have been transformed into three groups to promote better interactions. Two extramural efforts also are taking place: a marine bioscience and health program with the HML in Charleston, South Carolina, and work with the NCI on nanoparticle toxicity (nanoparticle toxicity work is also going on in the ACD). The BSD has formulated a set of strategic goals tied to the BioVision for NIST. Referred to as "mapping onto the omics," the overarching goal is to integrate the various activities of the division into the emerging fields of genomics, transcriptomics, proteomics, metabolomics, and cellomics. By focusing on how NIST can provide measurement science and standards to these disciplines, the division believes that it will be able to align itself effectively with key national priorities and optimize the impact of its expertise. Overall, the strategy is an excellent one and should serve as a solid template for assessing BSD's progress over the next few years.

ADDRESSING NATIONAL PRIORITIES

BSD has refocused its priorities to reflect the strengths that NIST can bring to the biotechnology enterprise. Health care and environmental issues; understanding basic biological mechanisms and translating this information into useful technologies; and incorporating new metrologies and standards into its mission are top priorities for the division. Because the U.S. Measurement System (USMS) was an important national priority and a far-reaching effort led by NIST, BSD should link its research more extensively into the findings of that recently completed study. A recent interdisciplinary team has completed an analysis of program opportunities in bioscience (biomarkers and systems biology) to understand and realign CSTL's bioscience priorities. The next step will be for BSD to get external input in order to make sure that its program choices will have maximal impact in the scientific community. The new strategic focus holds promise for significant progress in the next year.

IMPACT AND INNOVATION

BSD has a solid track record for high-impact, innovative research that seems to be highly fragmented. Its members have contributed to the development of a BioVision for NIST. The recent Program Opportunities Task Force has attempted to tie these excellent pieces together via a small set of overarching research objectives that would increase cross-fertilization and leverage to meet larger unmet measurement needs, ideally in conjunction with the findings of the USMS study. These goals might impact about 20 percent of the research agenda, still allowing for the majority of the portfolio to be composed of smaller-scale research investigations. However, in these areas, some degree of top-down objective setting could focus the contributions. Collaboration across entities exists but is mostly bottom-up and project-oriented. The new division leadership has all the right management and organizational skills to successfully drive this forward. In addition, the division operates with relatively small teams (two or three scientists). A greater impact could undoubtedly be achieved with fewer but larger teams focused on key problems.

The overarching themes that have emerged from recent strategic analysis are standards and technology for biomarker discovery and use and measurements, standards, and technology for understanding complex biological systems. BSD hopes to align its groups under these themes in order to achieve a high impact. This effort should be rapidly implemented. There are a number of programs that are innovative, well-motivated, and an example of NIST's unique mission and capabilities:

- The program on array scanner error and calibration across platforms represents good science that aligns with the mission of NIST. It represents a unique ability to understand and standardize measurement as new applications of arrays go beyond gene expression. This work should be extended, most notably to comparative genomic hybridization, copy number variation, and microRNA.
- The program on DNA damage and repair measurements demonstrates excellent research that has resulted from years of contribution addressing challenging problems; it is even more valuable today than was anticipated at the outset.
- The program on DNA forensics represents excellent and important research on fundamental questions important to application needs.
- The program on quantitative cell biology demonstrates an impressive approach to multiplexed cellular measurements and quantitative cell imaging. This work addresses important unmet needs and directions for cellular pharmacology and diagnostics.
- The program on spore reference methods consists of very important, relevant, and useful research for biodefense and related applications.
- The program on biothermodynamics demonstrates very impressive measurement capability and understanding of the fundamental science.

Some of the BSD's strong research programs may benefit from a shift in direction to increase their significance or improve their alignment with NIST's mission:

- The x-ray structural work is challenging research, but its only focus seemed to be the discovery of new structures, which seems better suited to academia. It is unclear how NIST gained value from this work.
- The research in understanding cellulose to glucose leverages NIST's strong biothermodynamics core competency, but it is unclear whether this research is best done at NIST. For example, perhaps the Department of Energy or the National Science Foundation might be better able to drive efforts to gain a mechanistic understanding.

- While the microfluidics technology work appeared to be strong, its integration with cell biology was weaker and could benefit from collaboration with a biologist. As a result the microfluidics cell efforts seemed to lack purpose and direction.
- Systems biology is a key direction for biosciences investment, and it is good that this program has been launched in the cell and tissue measurements group. This is a good example of an area where higher level goals could be set that would drive greater integration of efforts, especially across informatics/biocomputing and biology, which appeared not as tightly linked as they should be.

In general, success criteria for programs would benefit from improved clarity. Basic research and directed research aimed at advancing the distinct charter and role of NIST seemed uncoupled and at times at odds. Directed research cannot, of course, occur without a fundamental understanding of the challenges and trade-offs in the underlying science, but the BSD would be well-served to explicitly link its more basic research investments to the potentially important measurement-related outcomes that are envisioned for its research. Senior leaders at CSTL could provide greater context and vision to both postdoctoral staff and more junior staff on how their basic research efforts will impact NIST's mission in the long term—that is, the business value of the standards linked to their more basic efforts. In this sense, especially for the more basic work, it was not clear that success and its impact were well defined. A study that can be done with a government research grant at a university and that does not advance measurement science and technology should not be done at NIST.

BSD's dissemination of results and products follows traditional scientific lines with articles in peer-reviewed publications as the primary mode. BSD and CSTL should formulate and communicate a clear strategy for invention disclosure and patents to stimulate the commercialization by others of their technologies and products. They should consider active participation in such standards organizations as ASTM F04. BSD should reach out to the basic and applied biology communities, initiating workshops and conferences that publish their proceedings and building an industrial advisory board to assist in setting priorities.

TECHNICAL MERIT

The quality of the research staff and their commitment to executing and publishing cutting-edge research are impressive. The technical merit of most of the research programs was outstanding, and the journals in which its researchers publish are of high stature. Scientists in BSD average two papers per year in good journals, and many are internationally recognized for their research. It is clear that this generation of researchers upholds NIST's outstanding reputation for rigor in metrology, understanding, and control. CSTL is taking a broad approach to where it can contribute to standards. It has gone well beyond traditional areas for standards (e.g., it bottles precise chemical solutions) and is looking for nontraditional opportunities to advance the biosciences, such as work in databases; ontologies; and multiplexed, multivariate computation.

INFRASTRUCTURE

BSD leadership has appropriately created a flatter organization that integrates two of the five existing units into three main groups. This integration of microfluidics and CARB activities into the BSD will create greater opportunities for synergy and cooperation across the program. Having fewer and larger organizations also reduces competition inside the organization and allows for more free-flowing sharing of resources to address higher level priorities.

Facilities and equipment are excellent, especially at CARB, which is located at the University of Maryland and whose infrastructure appears to be directly linked to its facility investments. Given the physical separation of BSD and CARB, the former should pursue opportunities for cross-site engagement through additional efforts such as Internet seminars and meetings, minisabbaticals, and other cross-site research opportunities.

There are currently 57 staff members and 40 guest scientists in BSD. Given the number of projects being pursued, the scientists are clearly stretched, and the low ratio of technical staff to Ph.D. scientists means that most senior scientists operate with minimal technical support. New program goals will probably necessitate additional staff if the division is to keep pace with the rapid expansion of the biochemical sciences in the United States and the world.

CONCLUSIONS

BSD is clearly undergoing considerable revitalization, both organizationally and strategically. The creation of a BioVision for NIST is an excellent idea. To ensure successful achievement of its goals, division leadership must strive to bring in young scientists who are trained at the relevant scientific interfaces; this is critical in light of the fast pace of advances in the field. BSD should also settle on a small set of projects within the disciplines of genomics, transcriptomics, proteomics, metabolomics, and cellomics. The selected projects will serve as the basis for future evaluation of BSD’s progress.

Physical and Chemical Properties Division

SUMMARY

The activities of the Physical and Chemical Properties (PCP) division are central to existing and emerging national priorities, and some U.S. industrial and academic establishments rely heavily on PCP's efforts. There is an apparent lack of mechanisms for effective internal dissemination of results and for communicating between groups, projects, and divisions. It would be desirable, for example, to have weekly seminars attended by all division staff. PCP is productive and has considerable impact, as indicated by the number of users who access the products it makes available on the Web or who license the software; it would be useful to document that productivity and impact in a more systematic manner. PCP and CSTL as a whole should develop a strategic plan for managed growth, including recruitment, and identify areas of opportunity and areas for concern.

ADDRESSING NATIONAL PRIORITIES

The measurement of chemical and thermophysical properties; the systematic archival, assessment, and dissemination of relevant experimental data; and the establishment of standards are all aligned with the mission of NIST. These activities are central to some existing and emerging national priorities, and PCP excels at them.

The division consists of eight groups, three located at Gaithersburg and five at Boulder. The activities and products of each group are listed in Table 1.

IMPACT, INNOVATION, AND TECHNICAL MERIT

The Chemical Reference Data group is developing standard chemical identifiers (InChI) and data for molecular identification, both of which support the NIST mission. The Chemistry WebBook maintained by this group disseminates results to the public. The WebBook is accessed by thousands of researchers (25,000,000 hits to date) and is a valuable national resource that could be made even more valuable by being integrated with the products of other groups in the PCP and other NIST divisions. A means of retrieving data for a list of compounds rather than just one at a time would be very useful. The Mass Spectrometry Data Center is impressive, and the group is pursuing new directions in peptide and protein mass spectra. This product is widely licensed by instrument manufacturers to include in their data analysis software.

The Computational Chemistry group's activities are essential for validating data sets and for calculating properties that are difficult to measure. Computational chemistry is an important activity, and the theory group nicely complements the experimental activities of several projects, including that on real fuels. Efforts to quantify the accuracy of theoretical predictions are important, as is the reporting of this information. The new direction, aimed at using theory to improve peptide identification by mass spectrometry, is a positive one. Theoretical work in nanotechnology is timely and will become particularly relevant as NIST's efforts in nanotechnology continue to grow. It would be

TABLE 1 Summary of the Activities and Products of Each Group in the PCP Division

Group	Activities	Products
Chemical Reference Data (Gaithersburg)	WebBook database; mass spectrometry and chromatography data; International Chemistry Identifier (InChI).	Chemistry WebBook; Mass Spectrometry Data Center; InChI.
Computational Chemistry (Gaithersburg)	Computational methods validation and development; peptide mass spectrometry predictions; electron transport; nanoparticle properties.	Computational chemistry comparison and benchmark database.
Real Fuels Project (Gaithersburg)	Measure and evaluate reaction rate data for combustion and atmospheric models; global warming potentials.	Gas-phase kinetics database; atmospheric kinetics; ChemRate.
Thermodynamics Research Center (TRC) (Boulder)	Information system development for thermophysical properties; evaluate and estimate properties.	ThermoML (IUPAC); ThermoData engine; TRC tables; FloppyBook databases.
Properties for Process Separations (Boulder)	Advanced distillation curves; fuel decomposition kinetics; properties of explosives; trace components in fuel gas; chemical analysis.	Gas chromatography data (in WebBook).
Experimental Properties of Fluids (Boulder)	Measurement of thermodynamic and transport properties.	Included in RefProp, others.
Theory and Modeling of Fluids (Boulder)	Develop high-accuracy models for fluid properties; property evaluation and estimation.	RefProp; SUPERTRAPP; others.
Cryogenic Technologies (Boulder)	Refrigeration process models; cryogenic measurement techniques; pulse tube cryocooler; properties and process data.	Cryogenic material properties database; cryogenic flow calibration/tests.

desirable, however, to develop new initiatives in many-molecule calculations and force-field development, which would facilitate closer ties to the experimental efforts in fluid property characterization. The division should also pursue its own efforts in methods development, thereby ensuring its access to state-of-the-art theoretical chemistry methods. The Industrial Fluid Properties Simulation Challenge in its current form is imperfect; some restructuring is needed to turn it into a more relevant and constructive endeavor.

The Real Fuels Project group represents an important activity that is highly relevant to our nation’s energy policies. Activities in atmospheric kinetics are also important for environmental considerations. An authoritative set of Global Warming Potential values for atmospheric species should provide useful guidance to climate control efforts. Making kinetic measurements at actual combustion temperatures is a worthy endeavor; the data are important and will be used.

The Thermodynamics Research Center (TRC) group is essentially a data collection, analysis, and dissemination activity in which many undergraduate students are involved. A thermodynamic data evaluation project evaluates literature data, archives it, and makes it accessible to users for a fee. This appears to be an extremely useful and successful project. The division has worked hard to make data easily accessible. Charging for its use, however, is a barrier to dissemination. Dissemination to educational institutions should be free in order to maximize its value to the nation, and there appears to be a genuine desire within the division to do this. Commercial users should pay a fee that is commensurate with their user base. Overall this thermodynamic data evaluation project is an impressive activity.

The Properties for Process Separations group interacts extensively with industry. Sometimes collaborations produce funding, depending on the arrangement. This group includes an effort aimed at measuring the properties of explosives, including vapor pressures, surface energies, and permeation. It has developed clever techniques to measure very low vapor pressures, an essential attribute for work on explosives detection, which is sponsored by the Transportation Security Administration (TSA). This work is highly relevant and important. NIST seems to be one of the few agencies measuring these properties. It should advertise this function or activity and generate more resources for this work, particularly from TSA and other intelligence/security agencies. It would be desirable, moreover, to interact with detection instrument makers. Additional communications and possibilities for synergistic collaboration (e.g., with other national metrology laboratories) in this area should be explored. The Properties for Process Separations group also measures distillation curves, which provides a wide variety of information for applications. The group has developed a new concept called the Advanced Distillation Curve (ADC). This is essentially a more controlled and elaborate way of measuring distillation curves that reduces variability and uncertainty. Advanced distillation curves include much more information, including the composition of each fraction that is being distilled. This activity, while useful, is quite mature and not really at the forefront of research. More innovation is necessary, and it would be desirable to extend collaboration with the Real Fuels Project.

Experimental Properties of Fluids is a data acquisition group with considerable expertise in the measurement of thermodynamic and transport properties of pure components and mixtures (e.g., densimetry, phase equilibria, calorimetry, thermal conductivity, quartz-balance viscometry). Priorities for measurements are set by very reasonable criteria. Overall this is a solid group conducting state-of-the-art thermodynamic measurements. A new effort on biofuels centered around alcohol mixtures and biodiesel (esters from plants) is likely to produce useful results. The group's comprehensive activity will include data measurement and modeling to feed information to customers. An enhanced knowledge base will permit better evaluation of alternatives, more prospects, and better economics. This could become a high-profile project. The group should explore and establish connections to the Department of Energy.

The Theory and Modeling of Fluids group is relatively small. It includes multiple collaborations with overseas groups, including some in Germany, Japan, Greece, Great Britain, Argentina, and Mexico. Development of accurate equation-of-state (EOS) models for fluids, including refrigerants and significant components of combustion and synthesis gas streams, is important for technology advances in new refrigerants and novel energy systems. The RefProp computer program, which implements these models in an easily usable form, is an effective way to disseminate these results. EOS development or data measurement is declining in the United States and increasing overseas. The group expressed concern over a shortage in this country of individuals highly trained in data measurement and prediction. The emphasis of the group is on description-correlation of properties, as opposed to prediction. The modeling effort should be expanded and become comparable to the accompanying experimental program. True predictions are essential to gain insights, to design or engineer fluids with particular properties, and to provide properties for difficult systems (e.g., explosives, where the samples are allegedly very hard to get). The connection between the many-molecule theory efforts at the Gaithersburg facility and those at the Boulder facility should be strengthened. Activities in humid gases provided a noteworthy example of what can be done with true predictions and of how electronic structure efforts can be combined with statistical mechanics to address important experimental questions. PCP should consider expanding efforts along these lines.

The Cryogenic Technologies group activities include measurement, model development, calibration of cryogenic flowmeters, and materials evaluation (materials testing is no longer pursued at NIST, but literature continues to be mined and evaluated by NIST). The group focuses on advanced refrigeration systems, mostly closed-cycle coolers (sponsored by a variety of agencies or customers, including the Navy, the Defense Advanced Research Projects Agency [DARPA], the Air Force, and Cryomagnetics, Inc.). This is a creative group and represents a national resource for work on cryogenics. The efforts are clearly technologically relevant, and this advanced group offers unique capabilities.

Databases are part of the activities and products of several groups, including Chemical Reference Data, Computational Chemistry, the Real Fuels Project, Cryogenic Technologies, and the Thermodynamics Research Center. However, there is a need for a comprehensive plan for maintaining, improving, and disseminating critical, fundamental databases such as those for chemical kinetics and electron impact cross-section.

The number of talks presented by the PCP division at scientific meetings in 2006 (78 presentations) declined significantly (by more than 30 percent) from what it had been in recent years. It was unclear whether this was a result of budgetary restrictions. It is extremely important for the division staff and postdoctoral fellows to publicize their work at meetings.

There was an apparent lack of mechanisms for effective dissemination of results and for communication between groups, projects, and other CSTL divisions. It would be desirable, for example, to have weekly seminars that are attended by all division staff. This is particularly important since this division is split between two sites.

PCP must continue to publish its members' work aggressively. The number of publications in 2006 was consistent with that in previous years (an average of about 70). The number of publications is one of the key metrics by which engineers and scientists evaluate their performance, and it is important for PCP to maintain a high profile in the literature. It is also important for the division to examine the metrics that it uses to evaluate its progress.

INFRASTRUCTURE

The division has traditionally been a leader in the measurement, characterization, and prediction of thermophysical properties. The division has always had a well-deserved, outstanding reputation in academic and industrial circles. It must ensure that such a tradition of excellence is maintained, particularly as prominent senior researchers retire or leave NIST. Some in the division expressed concern that it is becoming increasingly difficult to recruit young scientists and engineers in the areas of interest to PCP. The division and the laboratory as a whole should develop a strategic plan for managed growth that would address recruitment issues and could identify areas of opportunity and areas of concern.

The division has access to state-of-the-art instrumentation. Part of the division, particularly in Gaithersburg, expressed concern about the lack of physical space for staff and laboratories. The laboratory should address that concern and develop and discuss its plan for more effective space allocation.

CONCLUSIONS

PCP activities are central to existing and emerging national priorities. Some U.S. industrial and academic establishments rely heavily on the efforts of the division. There were, however, few apparent mechanisms for effective internal dissemination of results or for communication between groups, projects, and divisions. It would be desirable, for example, to have an internal weekly seminar series attended by all division staff. The division is productive and has considerable impact, as indicated by the number of users who access products that the division provides on the Internet or who purchase licenses for the software; it would be useful to document that productivity and impact in a more systematic manner. The division should develop a strategic plan for managed growth that would address recruitment issues and could identify areas of opportunity and areas for concern.

Process Measurements Division

SUMMARY

The Process Measurements Division's (PMD's) mission of disseminating national measurement standards for thermodynamic parameters and conducting relevant measurement science research fits well with national priorities and NIST focus areas. PMD provides essential calibration services in fundamental parameters that support many sectors of the U.S. economy as well as facilitate international commerce. It conducts research that is directly aligned with NIST and national priorities. Examples include research supporting the Department of Homeland Security (microsensor chemical detectors), the climate change research community (spectroscopy, gas properties), the biopharmaceutical industry (gold nanoparticle reference material), developers of the hydrogen economy (hydrogen gas data and flow rate), and the semiconductor industry (atomic layer deposition, humidity, and trace gas measurements). In those parameters for which PMD maintains U.S. national standards and provides measurement services, it is generally preeminent among NMIs. This division is an important national resource. The overall mood of PMD staff appears to be positive, with researchers who are dedicated to maintaining and enhancing the international stature of the division.

ADDRESSING NATIONAL PRIORITIES

The NIST mission and current national priorities place increasing demands on technologies and services that are the responsibility of PMD. The technologies necessary for nanomanufacturing, the production of biofuels, enabling the hydrogen economy, development of clinical diagnostics and therapies, measuring climate change, and other national priorities can be developed no faster than the underlying process measurements on which they depend. Advances in temperature, pressure, humidity, material properties, and other fundamental measurement areas are essential to the exploitation of new technologies as well as to accomplishing the goals outlined in the American Competitiveness Initiative. For example, research is necessary in PMD parameters to keep up with the rapidly changing demands of nanotechnology. An array of technologies must be advanced to address homeland security issues, and these technologies will put pressure on process measurements and the underlying measurement science for which PMD is responsible. For example, evaluating climate change calls for significant improvements in the measurement of atmospheric parameters and better knowledge of the properties of atmospheric gases. To make practical use of hydrogen, accurate information about the gas (viscosity, speed of sound, flow rate, and the like) is needed.

IMPACT AND INNOVATION

PMD's goals include the following:

- Research to improve national measurement standards for temperature, fluid flow, liquid volume and density, pressure, vacuum, humidity, and airspeed.
- Developing the science base that supports new and improved measurements and standards technologies.
- Dissemination of measurement resources and technology through calibration services, SRMs, standard reference data, proficiency testing at the customer's site, and other means.

PMD has been improving measurement services and making them more automated. The division staff have reduced uncertainties in many parameters. For example, the measurement of gas viscosity is now accurate to ±0.08 percent in the range from 200 K to 400 K. Intermediate-range gas flow measurement uncertainty has been reduced from ±0.13 percent to ±0.009 percent. These improvements have benefited the semiconductor and gas flow instrumentation industries, among others. The new trace gas humidity system will measure to 14 ppb at ±1.8 percent uncertainty, a competitive advantage for U.S. producers of industrial gas and manufacturers of semiconductors. Hydrogen gas data are now available, with uncertainties of ±0.08 percent for viscosity and ±9 ppm for speed of sound. A new, less expensive calibration service is planned for completion in 2008 for mid-range vacuum calibration.

The potential impact of success in PMD research areas is also significant. U.S. dominance in nuclear technology, hydrogen technology, the application of biofuels, biopharmaceutical manufacturing, and nanotechnology will require major innovations and advances in the measurement technologies for which the division is responsible. A few examples of research programs that could have a very large impact are listed below.

- Because its performance is based on fundamental physical phenomena, the Johnson noise thermometer (JNT) could provide a means of placing temperature measuring systems within the cooling systems of next-generation nuclear reactors and in satellites, maintaining accuracy without needing to be removed for calibration. The same device has research applications that include improving the temperature scale, to which it is already being applied at NIST. The JNT technology will soon also be applied by NIST-Boulder to improve AC voltage measurements.
- In response to the needs articulated by the NCI, gold nanoparticle reference materials are being developed as part of CSTL's work on technologies for future measurement standards. Accurate cell phenotying requires quantitative analysis of images containing gold nanoparticles. In this connection, it is necessary to know that all the nanoparticles are of the same size and to know the specific size of the bare particle after each surface modification, which PMD researchers have demonstrated by a creative application of differential mobility analysis. Successful dissemination of gold nanoparticles as NIST

reference materials may facilitate new treatments for cancer and other diseases.

- Advances in gas concentration standards, spectroscopic relative intensity standards, and in measurement of pressure, temperature, and humidity—all of which are active programs in PMD—will improve the monitoring of climate change and will support semiconductor manufacturing as well as a wide range of other desirable objectives.
- More accurate property data for hydrogen (speed of sound and viscosity) will be used in a number of applications essential for moving the nation to a hydrogen economy.
- Chemical sensors using PMD-developed microhotplate technology may make possible reliable alarms for poisonous gases under real-world industrial and military conditions.
- PMD is developing models and metrology techniques for plasma-based processing of semiconductor devices such as atomic-layer deposition of high-k dielectrics for next-generation transistors.
- The hybrid humidity project, nearing completion, takes advantage of the expertise and scientific knowledge about humidity that is uniquely available in PMD, including operational knowledge gained by operating the U.S. national standard for humidity.
- The atomic standard of pressure program is attributable to PMD's expertise in resonant acoustic and millimeter-wave techniques for determining gas properties. At present the system may demonstrate within months its potential to revolutionize pressure calibration by replacing piston gauges as primary pressure standards.
- PMD is a leader in the area of micromachined chemical sensors. Especially noteworthy is the division's demonstration that arrays of microsensors can recognize low concentrations of toxic industrial compounds in high background levels of reactive interferants. Applications for this technology include chemical warfare agent detection on the battlefield.
- A new instrument, dubbed the "whispering gallery" resistance thermometer and based on the properties of sapphire, is being developed as a means of measuring temperature without relying on mechanically fragile platinum resistors.
- The National Aeronautics and Space Administration has requested a calibration database of the chemical species involved in determining the dynamics of CO_2 in the atmosphere. PMD-developed cavity ring down spectroscopic measurements will provide these spectroscopic parameters at the required ±0.3 percent uncertainty level for the 2008 launch of the Orbiting Carbon Observatory, designed to monitor global climate change.
- A comprehensive, three-tiered proficiency testing program in temperature has been implemented to support customers from the highest level (standard platinum resistance thermometers) to the factory level (thermocouples). To maintain accreditation, proficiency testing support is essential for commercial laboratories that perform calibration. This new service is advertised in the *Bulletin of the National Voluntary Laboratory Accreditation Program*.

TECHNICAL MERIT

In most calibration and measurement areas, the PMD has superb measurement capability, and it maintains this capability through continuous process improvements and research. One example is the ultrasonic interferometer manometer, which is used to produce the best primary standard of pressure. Since moving to the Advanced Metrology Laboratory it achieves an uncertainty of 3 ppm in a room whose temperature is controlled within ±0.1°C. These measurement capabilities are foundational to U.S. competitiveness, especially in new and emerging technologies. The large number of publications, committee leaderships, and visiting U.S. and foreign scientists and postdoctoral fellows testifies to PMD's technical reputation and leadership position in measurement science.

Many of the division's measurement capabilities are among the finest of their type, as reflected by both informal and formal key comparison analyses conducted by NMIs for the primary pressure standard (CCM.P-K4 and -K5), liquid volume (CCM.FF-K4), natural gas at high pressure (CCM.FF-K5.a), and compressed air and N_2 (CCM.FF-K5.b). PMD continues to develop and initiate new calibration services (e.g., for humidity and trace humidity in 2006).

In FY06 division researchers produced 55 manuscripts for publication, had 30 manuscripts accepted for publication, made 94 presentations, produced 6 patents, and participated on 73 committees, generally as committee leaders.

INFRASTRUCTURE

In a number of areas the division experienced declines in full-time equivalent (FTE) positions, such that Ph.D.s charged with essential calibration missions do not have sufficient time for research because they do not have enough technical support staff. The risk of continuing along this path is that Ph.D. researchers will either leave NIST or lose the expertise necessary to advance metrology. There is a need to maintain proficiency and competency in developing standards; a calibration laboratory cannot be sustained with technicians alone. A continuation in the decline of FTEs will necessitate cuts in calibration services and have negative repercussions for U.S. industry and commerce. CSTL should consider applying a differential cost recovery system for calibration services and a new fee system for these services within the federal guidelines governing NIST's mandate.

CONCLUSIONS

PMD plays a key role in accomplishing the NIST mission, which is unique and differs from that of academia, commercial, and other government research organizations in that it focuses on measurement science, the development of metrological tools, and calibration standards. Its resources include experts in specific technical areas along with some of the best measurement and calibration systems. Together, these resources give PMD unique capabilities and strengths that are reflected in the wide range of research programs and measurement programs in which it is involved.

Better PMD calibration services enhance U.S. competitiveness, promote science and technology, and further the NIST mission. The Department of Defense, Department of Homeland Security, Department or Energy, and U.S. industry depend upon NIST to define measurement uncertainties and to serve as the legal link to the International System of Units.

Surface and Microanalysis Science Division

SUMMARY

The work of the Surface and Microanalysis Science Division (SMSD) is on a very high level, and the clear dedication and focus of its staff are very impressive. The SMSD seemed to meet all of the objectives that had been set before it.

ADDRESSING NATIONAL PRIORITIES

SMSD pays great attention to both national and NIST priorities, with the Department of Homeland Security receiving a significant amount of attention. A highlight of this work is the superb project on the identification of small quantities of explosive materials in an airport environment. The challenges are enormous, but the SMSD has met them admirably. The work on the detection of explosive materials transferred from fingers to fingerprints on surfaces is particularly impressive. SMSD has also made strides in the study of reproducible swiping of luggage surfaces as a sampling method. There appears to be a lack of theoretical support for this effort, however. Given that the mechanics of transport is such an important issue, such support would be invaluable in solidifying a very important effort.

Another example of how the SMSD responds to national priorities is the utilization of secondary ion mass spectrometry (SIMS) for the detection of enriched uranium in samples submitted by the International Atomic Energy Agency.

The SMSD has also made the important observation that the production of nanoparticles, a well-known scientific priority and growth area, may have important safety implications. This project, however, may not be as well defined as it could be and may need additional support.

IMPACT AND INNOVATION

The development of trace explosive standards based on the process of ink-jet printing was particularly innovative and satisfies the fundamental standards development responsibility of the laboratory. Although not SRM-based, it is making a big contribution to the calibration and verification of the many detection devices that are now or soon will be located in airports. This work directly supports Presidential Directive HSPD-19 on homeland security and will directly impact airport operations.

The SIMS program allows quantitative verification based on the analysis of very small samples of whether or not an inspected facility is producing highly enriched uranium. It allows determining whether a particular facility has been used to develop a nuclear program and as such is an important program.

The SMSD works on some long-range projects such as small-particle detection and analysis, which will have great relevance for the health and safety issues surrounding nanoparticles in the environment and for airport and port security.

TECHNICAL MERIT

The SMSD exhibited quite a few areas of excellent technical merit. One example is the work of the Microanalysis Research Group. The recent acquisition of a monochromated, aberration-corrected (scanning) transmission electron microscope puts the group at the leading edge of analytical electron microscopy. It will allow SMSD to do state-of-the-art chemical imaging on a very small sample. Recognizing the need for this kind of instrumentation, the division has assigned some extremely talented and widely known and respected staff members to its operation and development.

The workers in the SMSD have advanced the science of microscopy a great deal. Through the use of state-of-the art programmable optical elements and structured laser illumination sources, they have extended the light microscope beyond the well-known diffraction limit. This very valuable approach is far from an inexpensive add-on to a standard microscope. Making this instrument available to academic and industrial scientists would guarantee that it maintains its leading position.

SMSD is well known for its past work in X-ray Photoelectron Spectroscopy and has ongoing research activities using sum-frequency vibrational spectroscopy; this work is an important support for research in the field of spectroscopy.

The SIMS project involving the analysis of organic depth profiles using cluster ion bombardment is very important work, but it would profit quite a bit from stronger attempts to understand the theoretical basis for the excitation process and why some organic layers deviate from the norm.

While the work in molecular electronics is important, it has yet to lead to substantial results, which is a common problem in the field of molecular electronics. Moreover, it will probably not succeed without considerable additional support from experts in synthesis as well as experts with a better grasp of the theory, including aspects of self-assembly, device physics, and modeling. Additionally, connections to device fabricators and clean room operations are highly recommended. Without these additional resources, the work in molecular electronics may not attain significance.

SMSD has created databases to support surface analysis via electron spectroscopy; it should strive to maintain this valuable work well into the future.

SMSD has a very strong program in the analysis of small particles. The automated scanning electron microscopy (SEM)-based particle analysis allows for sizing up to 50,000 particles per hour and for quantifying 3,000 particles per hour. This work has enormous importance in semiconductor manufacturing and the analysis of particulate impurities and explosive materials in the air. These high-throughput methods add greatly to the data-mining capabilities of the division.

SMSD has recognized the importance of evaluating the health and safety risks of nanoparticles. This work would be better served if it were done in a clean room. Nanotechnology is a major thrust for the future, and a knowledge of its risks is clearly important. The production of nanoparticles standards is within the purview of the SMSD, and this work could lead to future SRMs.

INFRASTRUCTURE

SMSD's move to its new, state-of-the-art building, coupled with the acquisition of new equipment, was thought to be a predictor of further successes. However, it now appears that division personnel will be forced to move to other facilities. The CSTL should work with NIST management to analyze the costs and benefits of these rearrangements.

The policy of hiring many postdoctoral employees for limited terms is an excellent way to always have new ideas circulating within the division. The best of these employees could become permanent researchers for the division and would allow for the continuation of important projects after some current workers retire. This continuity is extremely important, and this aspect of the division's approach to future hiring is an excellent one. The large number of projects sponsored by the ion mobility spectrometry work attests to the liveliness and timeliness of its research activities.

Collaboration with other CSTL divisions is the norm and a signature of this division. If the collaboration can be extended to groups at universities or to other national laboratories, CSTL's work would have more impact on the scientific community.

The staff of the division is of high quality and spans many disciplines. This is an excellent factor contributing to scientific progress. However, more technician-level support would bring additional progress.

With the move into the new building, the division was able to improve its instrument suite; as a result, capital needs at this time are not dire. Although manpower issues are ever-present, SMSD does not seem to be struggling in its endeavors.

CONCLUSIONS

The quality of the division's work and its staff are on a very high level, and the dedication and focus of the staff are very impressive. The SMSD seems to be meeting all of the objectives that have been set before it.

Conclusions

CSTL is meeting its obligations, and its priorities are appropriate and aligned with national priorities. The technical merit of the laboratory and the commitment of the staff are high. There is no evidence that any programs are jeopardized by a lack of facilities or equipment. Future assessments will be facilitated if greater emphasis is placed on clarifying the distinctions between work performed to provide services and work performed to support research and development.

Against this backdrop of clear and consistent success and high technical merit, the panel makes several suggestions for improving the operation of the Laboratory (see Summary).