Developing a vision for the infrastructure and facility needs of the materials community: Report of NSF Materials 2022
(*A Subcommittee of the Mathematical and Physical Sciences Advisory Committee*)

July 2012

Introduction and Motivation

As previous reports on instrumentation and facilities have noted, the importance of analytical and imaging tools can scarcely be overestimated in the profound effects they have had on the advancement of science and human understanding of the world. The materials research community finds itself now at a critical juncture where access to instrumentation and facilities is limiting progress and competitiveness in U.S. materials research. New investment is needed, as is an approach that provides broader access to small and mid-size facilities. The National Science Foundation Division of Materials Research (NSF DMR) bears a particular responsibility in enabling such investments and access.

The Mathematical and Physical Science Advisory Committee (MPSAC) and NSF formed the Materials 2022 Committee to gather and synthesize community input, and to help DMR and NSF more broadly address challenges faced by the materials research community in the coming decade. Our report proposes guiding principles as well as actions for making new investments and achieving an optimum balance among investments in different scales of instrumentation and facilities.

Charge to the Subcommittee

NSF Materials 2022 will help develop a vision for the facilities and instrumentation needs of the materials community in the coming decade. This group will address comments made by the DMR Committee of Visitors (2011). The scope will include the following:

- How can the Division of Materials Research (DMR) best utilize its resources to meet national needs in instrumentation as well as provide access to unique instrumentation capabilities through user programs at national facilities?
- What is the best way to handle acquisition of multi-user instrumentation for the materials community, including operations and maintenance, taking into account instrument acquisition programs supported by other Federal agencies?
- What are the opportunities for development of new instrumentation and facilities, taking into account existing national user facilities, NSF's mission of transformative research, as well as the international context?
- What are the needs for workforce development (including undergraduate, small, minority serving, or geographically disadvantaged institutions) in these areas? How can DMR best utilize its resources to meet these needs?
- What is the recommended course of action considering the finite budget and staffing resources of DMR?

The following boundary conditions should be adopted:

- The committee will not consider proposals for future individual projects nor will it determine how funds are to be distributed among individual ongoing development efforts, but rather identify resources that can be distributed to these future efforts through DMR's normal review and priority setting processes.
- The committee's deliberations should take into consideration systemic issues such as U.S. scientific leadership within a global context, filling critical niches in the overall U.S. system, and the needs for training and technical innovation.
- Recommendations should be based on well- understood criteria established by the committee and articulated to the community.
- There should be opportunity for community input. Recognizing the brief time span of the subcommittee, web-based communications with the community are acceptable.

Background

The mission of the Division of Materials Research in MPS is to enable new discoveries about the behavior of matter and materials; to create new materials and new knowledge about materials phenomena; to address fundamental materials questions that often transcend traditional scientific and engineering disciplines and may lead to new technologies; to prepare the next generation of materials researchers; to develop and support the instruments and facilities that are crucial to advance the field; and to share the excitement and significance of materials science with the public at large. In order to accomplish this mission, the Division dedicates its resources to individual investigator and small group awards (largely through eight sub-disciplinary programs), education awards, a centers program, and facilities and instrumentation.

The goal of the facilities and instrumentation portfolio is to provide next generation approaches to enable the materials community to explore how electrons, atoms, molecules and their assemblies behave, with the goal of understanding the relationship between structure and properties and how to manipulate them such that systems with unique properties may be derived. We need to have the capabilities to not only probe and measure the properties but to be able to synthesize and process new material systems.

Currently through the Office of Materials Instrumentation and National Facilities (OMINAF), DMR serves as steward of two national user facilities, the Cornell High Energy Synchrotron Source (CHESS) at Cornell University and the National High Magnetic Field Laboratory (NHMFL) at Florida State University. It has a partnership role in facilities such as the Center for High Resolution Neutron Spectroscopy (CHRNS) at NIST, the National Nanotechnology Infrastructure Network (NNIN) and ChemMatCARS at APS. As for instrumentation, DMR supports the R&D, conceptual

design and/or construction of midscale instrumentation by/for the materials research community through its Instrumentation for Materials Research - Major Instrumentation Program (IMR-MIP). Acquisition of smaller multi-user instrumentation is supported by the **Instrumentation for Materials Research (IMR) program**. Through the Materials Research Science and Engineering Centers (MRSEC), it supports clusters of instrumentation available to centers members and outside users via the Material Research Facilities Network.

Subcommittee Membership

Roger Falcone	(UC Berkeley) co-chair
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Introduction

The Materials 2022 Subcommittee adopted a structure for the task of developing a vision for the infrastructure and facility needs of the materials community. The **goals** for NSF support of materials research instrumentation and facilities were discussed and formulated. Effective support **mechanisms** to meet these goals were examined and proposed. An analysis of **balance among alternatives**, that is, different scales and balances among various **components** of the materials research infrastructure, as they pertain to instrumentation and facilities was made and is presented.

Goals

In creating structure-property-composition relationships, from bulk to surface, from fundamental science to applications, progress in condensed matter and materials research is inextricably linked to advances in instrumentation. Indeed, advanced instrumentation is a principal driver of progress in materials science. International competition in materials research is very strong and correlated with regions of economic success; China, Singapore and Germany, for example, are making a variety of very substantial investments in materials research facilities.

Therefore, the over-arching goal of DMR must be to ***provide sustained financial investment that makes cutting edge instrumentation, especially essential, new and unique instrumentation, accessible to university-based research programs***. To drive the scientific agenda and sustain US leadership in the materials sciences, DMR must promote continued innovation and improved performance across the full spectrum of instrumentation. These developments impact other natural sciences including chemistry, biology, medicine, geology, and metallurgy and drive progress in synthesis and manufacturing that underlie technological renewal. Scientific discovery may be viewed by some as more glamorous than invention of new tools, but these two endeavors must be advanced in concert. The DMR instrumentation program is important to promote the academic stature of instrumentation development and attract new talent to this aspect of materials research. Specifically, DMR should ***promote research on development of new instrumentation that advances experimental frontiers, maintains an inventive culture and enables new discoveries***. Mass production is ultimately critical to expanding instrumentation access and achieving scientific and technological impact. NSF can play an important role in connecting academia to the private sector to enable commercialization of instrumentation of broad utility.

As the scope and diversity of materials research problems grow, the tools necessary for materials science increasingly includes instrumentation that cannot be acquired or maintained locally. Therefore, an important goal for DMR should be to ***enable access to unique experimental capabilities that are beyond the scale of individual investigator laboratories***. From medium to large-scale facilities, DMR must be engaged, along with the PIs, since access and continued innovation in instrumentation drives scientific output and is essential for continued US leadership in materials science. Midsize facilities provide access to instrumentation with acquisition costs ranging from $500k to $5M. NSF has successfully adopted a network access model, as exemplified by the National Nanotechnology Infrastructure Network (NNIN). ***A significant expansion of this type of model, tailored to the needs of the materials research community, is needed to cover a full range of equipment capabilities for materials synthesis, characterization and processing***. Large-scale facilities provide access to neutrons, intense x-ray and light sources, and high magnetic fields. Other agencies (notably DOE and DOC) operate most of these facilities, but NSF-funded individual investigators represent a dominant fraction of the user community with access through peer review. In this realm, relatively modest NSF investments can have disproportionately large effects on accessibility for users and their engagement in large-scale instrumentation development projects. The operations and maintenance of large-scale facilities benefit from a user base that is well supported, both for their principal research goals and for access to the tools needed to pursue them.

When a large-scale capability that is essential to materials science is not available through one of the mission agencies, DMR can and should reasonably take some responsibility for facility construction and operation; for example, the National High Magnetic Field Laboratory, which provides unique world leading capabilities for DMR PIs. It may also be the case when new forms of large-scale instrumentation become possible in the future, as exemplified in NSF's important historical role in the development of synchrotron sources. As a ***major sponsor of graduate education, NSF also plays a crucial role in the education of successive generations of facility users and***

operators. This role extends beyond traditional graduate education to encompass workshops and summer schools focusing on specific types of facility instrumentation.

Access to a rapidly evolving suite of instrumentation valued at $10K - $1M for the broadest possible range of active scientists has a very direct impact on NSF-DMR research productivity. NSF has a role in development of new instrumentation capabilities, transition to commercialization, acquisition, maintenance, education and training. Further investment to ***provide access to a full range of cutting edge commercial instrumentation is very much needed***. Maintenance, reconfiguration, and upgrades to existing instrumentation can greatly enhance research productivity and should be a more substantial part of DMR's role in instrumentation. Whether a given type of instrumentation best resides in a PI lab or in a recharge multi-user facility depends not only on the cost but also on the modality of the experiment. DMR has a general interest in assuring instrumentation investments in this range are employed for cutting edge materials science to the fullest extent possible.

Summary of **Goals**: The charge to the Materials 2022 Subcommittee was, in part, to develop a compelling vision for the science and broader impacts for instrumentation programs and partnership/stewardship of national user facilities. To that end, the appropriate goals for a successful program of investments in instrumentation and facilities are:

- ***To provide sustained financial investment that makes cutting edge instrumentation, especially essential, new and unique instrumentation, accessible to university-based research programs***.
- ***To promote research on development of new instrumentation that advances experimental frontiers, maintains an inventive culture and enables new discoveries***.
- ***To provide access to a full range of cutting edge commercial instrumentation***.
- ***To provide geographically distributed access to a full range of equipment capabilities for materials synthesis, characterization and processing***.
- ***To play a crucial role in the education of successive generations of instrument and facility users, developers and operators***.
- ***To enable access to unique experimental capabilities that are beyond the scale of individual investigator laboratories***.

Mechanisms

Characterization equipment and facilities are paramount to advancing the state-of-the-art in materials research. US universities face considerable challenges in obtaining instrumentation and associated facilities, funding operational expenses, and attracting/retaining expert technical staff essential to the conduct of advanced, cutting-edge research. Furthermore, differing clientele, educational roles, and budgetary constraints make it impossible to devise a "one size fits all" model for best practices. Nevertheless, there exists a need to develop models that maximize the effectiveness of the education and research missions of these capabilities, while communicating the importance of such equipment and facilities in national education and research goals.

The 2006 National Research Council Report on Midsize Facilities (the Sinclair report) had five major recommendations; Collective Stewardship; Regional Networking; Long-term Infrastructure; Professional Staffing and Periodic Review. These recommendations, many of which have not been addressed in detail, are more relevant today than they were 5-6 years ago. The cultural shift in the community to a model based on sharing is growing. The influence of the Internet and the ease of remote access, are powerful in their potential to impact the future of all DMR research significantly. In addition, the diversity and geographical distribution of academic and industrial research groups conducting materials research continues to grow with many areas of the country having reduced access to local instrumentation and facilities. The Sinclair report also anticipates (perhaps provoked) some of the major recommendations of the 2011 DMR COV report, with the following recommendation being particularly relevant: "*DMR should develop instrumentation networks, possibly a national network, along the lines of the Materials Research Facilities Network (MRFN) developed by the MRSECs"***.**

Multiple reports presented from 2002 onward (including the 2011 DMR COV report) outlined the increased need for national attention to stewardship of instrumentation and characterization facilities. Developments in the institutional and national support of such facilities have not adequately reflected the growing needs of the research community for access to high-level instrumentation. These major issues are also coupled with increasing capital cost for acquisition and increasing physical and technical support needs. With this increased demand and changing profile for needs in research instrumentation, the call for managed facilities of shared equipment with dedicated technical support staff have increased, often replacing instrumentation for individual PIs and research groups, who cannot maintain the facilities or expertise to support increasingly advanced equipment.

Recommendations on mechanisms of support are grouped into three categories: Roles and responsibilities; Collaboration, sharing and access modes; Stewardship.

Roles and responsibilities

Recommendation: *DMR should increase funding for MRI proposals and develop a mechanism for the acquisition and stewardship of equipment in the $100,000-$500,000 range, in addition to a (smaller) number of mid-size equipment (500K-5M$ range), and allow for the possibility of bundling smaller pieces of equipment together in a single proposal to fulfill a suite of related characterization problems*. Critical components in this effort also include the training of users, availability to outside users and long-term viability of equipment. Plans for these components should be among the criteria for funding.

Recommendation: *DMR should recognize and facilitate the critical role that professional staffing plays in the successful operation of instrumentation and characterization tools*. Models/programs should be developed that allow for this impact to extend over the full DMR portfolio. A key issue here is the long-term career structure offered to academic professionals, PhD level scientists who are most effective in providing the continuity of expertise needed to support sophisticated equipment, such as semiconductor clean-rooms or advanced electron microscopes. It is vital that our

universities provide such a long-term career structure for these crucial people. A mechanism for reasonable job security, such as multiple-year rolling contracts, may be needed if these positions are funded from soft money or user fees.

Recommendation: Historically, the observation of a new effect in physics (e.g., NMR, lasing, ion sources, Raman scattering, magnetic lenses, Bragg scattering, electron tunneling) has been followed by a gestation period of up to a couple of decades before a useful materials characterization instrument appears. If new instruments are to appear in the United States based on entirely new principles, *it is crucial that small-scale funding be provided to instrument developers during this gestation period of University-based research, before commercial interest is attracted.* Recent examples include the X-ray laser, the new super-resolution optical microscopies, the STM, ion sources and aberration-correction in electron microscopy.

Collaboration, sharing and access modes

Recommendation: *DMR should act on the long-standing idea originally from other sources, advanced here again, to develop a network of centers, termed Materials Discovery Centers (MDC).* These centers may focus on either the provision of a broad instrumentation portfolio to the external community or to fulfill a specific need/expertise (i.e. X-ray, microscopy, crystal growth). Critical features of the MDC are a focus on professional staffing for training, user support, research and education. Viable and successful models include the NNIN and MRFN where capacity and utilization is very high. The DOE nanocenters provide another useful model; indeed, collaboration with DOE in some aspects of these endeavors is worthy of exploration. These MDC should be spread geographically and could be derived from existing efforts (i.e. University central facilities, MRSEC Shared Experiment Facilities, multi-user facilities, etc.) as well as new centers – would be based on a new solicitation. Focus would solely be on the provision of state-of-the-art equipment and characterization facilities both from a research as well as an educational viewpoint. This focus will allow other DMR programs to get back to their core missions in research and education.

The advantages of a portfolio of Materials Discovery Centers are numerous and compelling. MDC's would provide a fertile environment for equipment development and preliminary evaluation of new characterization tools suitable for wider usage. Significant leveraging of expertise in equipment operation, training, maintenance, etc. would be expected. The MDC's could create a successful model for utilization and maintenance of MRI-supported equipment well beyond the initial funding period. Base funding to MDC's could allow a route for equipment in the critical $100,000-$500,000 range that is difficult to obtain via other means. MDC's would also benefit from equipment made available through other funding sources. The availability of professional staffing would allow for the optimal operation and availability for all instrumentation purchased, not just DMR-derived equipment. MDC User fees could provide a mechanism for sustaining equipment and characterization tools. The business model for managing multiple pieces of instrumentation would be simplified *via* centralization. The diversity of a MDC program ("one size *doesn't* fit all") would allow a greater balance in terms of support for research universities, undergraduate and minority-serving institutions. Significant impact

on industry would also be expected. MDC's should be dynamic and provide for close out of facilities and the establishment of new facilities.

Recommendation: *Investments in instrumentation and facilities should be well aligned with national initiatives*. Funding of instrumentation and characterization tools provide for powerful synergies, for example, with the Materials Genome Initiative. Funding could be used to promote strategies to standardize the sharing of data, data format, libraries – users should also be encouraged to share raw data. Over time, DMR support could be used to build a capability for comprehensive data collection, as with crystallographic databases. This capacity is very difficult to achieve without a centralized mandate or through the efforts of a national network such as the proposed MDC's.

Stewardship (acquisition, operation, maintenance, evaluation, closeout)

Recommendation: *DMR must consider the stewardship of instrumentation to be as important as the acquisition of the equipment*. Follow up data and usage statistics should be part of any proposal related to equipment.

Recommendation: *DMR should recognize the need for the expanded usage of equipment and facilities beyond the PI's host institution. Promotion of equipment availability, capabilities and usage information is key*. Again the MDC could play a key role. A database could be developed for all equipment managed and operated by the MDC's – however the MDC could also have the added responsibility for collecting data from successful MRI proposals in their region. For this to be successful, the DMR should require PIs to work with the MDCs in this regard.

Summary of Recommendations on **Mechanisms**:

A major investment in instrumentation for materials characterization is needed, with an initial significant investment for multiple years to catch up with deferred investments, and a continuing and sustained investment to build and make available to the community the next generation of world-leading instruments. An initial surge in funding is critical to establish a vibrant program. Technical staff to upgrade and maintain the state of the art instruments and to train users is critical. This stewardship task cannot be left to students and postdocs. The instrumentation proposal should be linked to national strategies for science, technology, innovation and competitiveness where appropriate. Advanced and innovative instrumentation is a primary enabling capability, central for NSF to achieve its research and education missions. The investments here are essential for continued health and international competitiveness in materials science and engineering.

- ***DMR should increase funding for MRI proposals and develop a mechanism for the acquisition and stewardship of equipment in the $100,000-$500,000 range, allowing for the possibility of bundling smaller pieces of equipment together in a single proposal to fulfill a suite of related characterization problems.***
- ***DMR should recognize and facilitate the critical role of professional staffing in the successful operation of instrumentation and characterization tools.***

- ***It is crucial that small-scale funding be provided to instrument developers during a period of University-based research, to keep a pipeline of new instrumentation flowing.***
- ***DMR should act on the long-standing idea originally from other sources, advanced here again, to develop a network of centers, termed Materials Discovery Centers (MDC).***
- ***Investments in instrumentation and facilities should be well aligned with national initiatives.***

Balance Among Alternative Components of Instrumentation and Facilities Investments

This report has thus far pointed out some critical needs and made recommendations on where new investments should be made in smaller scale instrumentation, better access to instrumentation, new instrument development, staffing, and a new networks of Materials Discovery Centers. The case for all of these investments is very strong but it is not the entire picture. How to accomplish this in an environment that also includes DMR funding for major user facilities must also be considered, not only from the point of view of funding decisions, but perhaps more importantly, from a policy point of view. What should be the priorities of NSF DMR be in the provision of the entire spectrum of instrumentation and facilities, from smaller to larger scale?

This Subcommittee discussed alternatives extensively. While it did not feel able to make a detailed recommendation on funding balance across this spectrum, there was reasonable consensus on the policy side, that is, on the philosophy of how DMR equipment and facilities investments might best be made. This can be distilled in to two statements: ***(1) More investment needs to be made to enable excellent access, utilization and development of instrumentation from the small to mid-size, as defined earlier; DMR has a special responsibility to foster the earliest stages of research into effects that are likely to lead to characterization tools based on entirely new principles. (2) Large-scale facilities investment by NSF should occur if a convincing case is made that the facility provides unique capabilities, not available elsewhere.***

There is a general feeling that the US is falling behind in its investment related to point (1) above and that it is vital that this trend be reversed. On point (2), the Subcommittee heard from many users of large-scale facilities about the important role they, too, play in advancing materials research. There is no argument about that. The discussion should be more centered on the proper role of NSF, as compared to DOE, NIST and other agencies. The Subcommittee opinion is that NSF should value uniqueness and novelty over capacity building in large facilities as criteria for support. NSF should also emphasize the importance of education of the next generations of instrument scientists and expert users of materials research facilities in making decisions on where to invest its financial support.