

More Data at DMR: MIPs, DMREF, and Beyond

Eva M. Campo

Division of Materials Research, National Science Foundation

MRSEC Directors meeting, October 2018



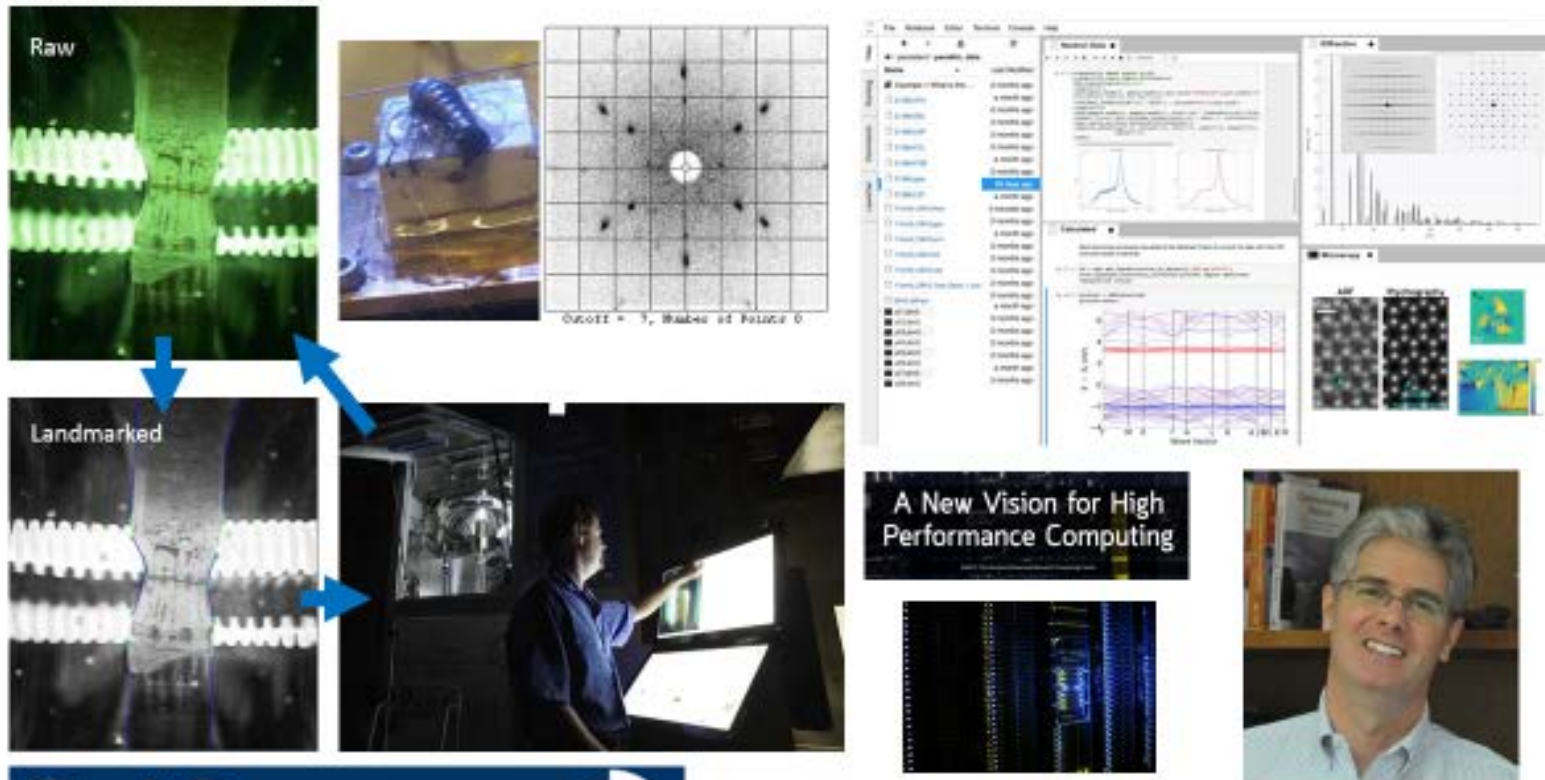
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PARADIM Data Availability and Usability



“Collect Everything,” “Use everything,” “Make available everything”

Machine Learning



SciServer

idies

nanoHUB

Developments

- Introducing DMR Data pilots:
 - NSF- 2D Data Framework- DMREF+EFRI+MIPs featuring Google Cloud Services
- DMR Data Working Group
- AAAS Fellow
- Data and Diversity: PREM and more
- Tripods + X
- DCL- Data Reuse
- Data in X-Cutting
 - Intervention through multiple Big Ideas: Microstructure

Proposals that align with NSF's Big Ideas are encouraged, but not required.

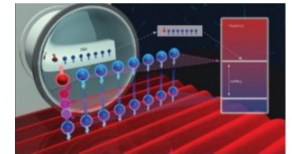
Harnessing Data



Shaping the New Human Technology Frontier



Quantum Leap



Understanding the Rules of Life



Navigating the New Arctic



Windows on the Universe

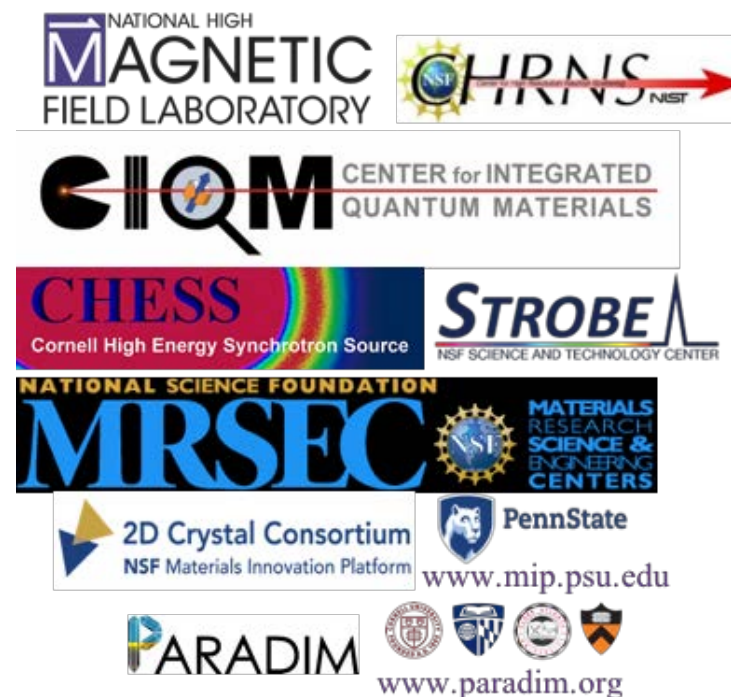


https://www.nsf.gov/about/congress/reports/nsf_big_ideas.pdf



DMR-supported centers and facilities

1. Materials Research Science and Engineering Centers (MRSEC). <https://mrsec.org>
2. Science and Technology Centers (STC). <http://ciqm.harvard.edu> and <http://strobe.colorado.edu>.
3. Materials Innovation Platforms (MIP). <http://www.mri.psu.edu/mip> and <https://paradim.cornell.edu/>
4. National High Magnetic Field Laboratory (NHMFL). (<https://nationalmaglab.org/>)
5. Cornell High Energy Synchrotron Source (CHESS). <http://www.chess.cornell.edu>
6. Center for High Resolution Neutron Scattering (CHRNS). (<https://www.ncnr.nist.gov/programs/CHRNS/>)



Material Innovation Platforms (MIPs)

NSF-DMR currently funds two MIPs that operate under the MGI philosophy.

Concept: Combine a **focused research effort** in an interactive feedback loop together with a **mid-scale user facility open to the community** in order to accelerate advancement of a materials research topic of national importance.



Focus: 2-dimensional chalcogenide materials for future electronics.
e.g., Can theory model growth kinetics and guide materials synthesis?



Focus: Interfacial materials, combining oxides & 2D materials, for valleytronics & spintronics
e.g., Can we design and create new interfacial materials by “breaking” Gibbs’ & Pauling’s rules?

Current Status:

- Accepting user proposals; some samples already delivered to users
- World’s first 300-atm floating-zone furnace at Paradim-JHU →
- Integrated MBE, CVD, ARPES & STM/AFM
- Access to computational, TEM & other capabilities
- Webinars and summer schools



Report on 2D Materials & Devices Data White Paper Competition



PennState



EFRI-2DARE, DMREF-2D, and MIP Grantees Meeting

Accelerating Research in 2D Materials and Devices

A Team Building Exercise for the Engineering and Materials Community

DMR Data Working Group



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Event at a glance

Held at Penn State's MIP

2DCC focusses on 2D chalcogenides for applications in next generation electronics for digital circuits and flexible electronics

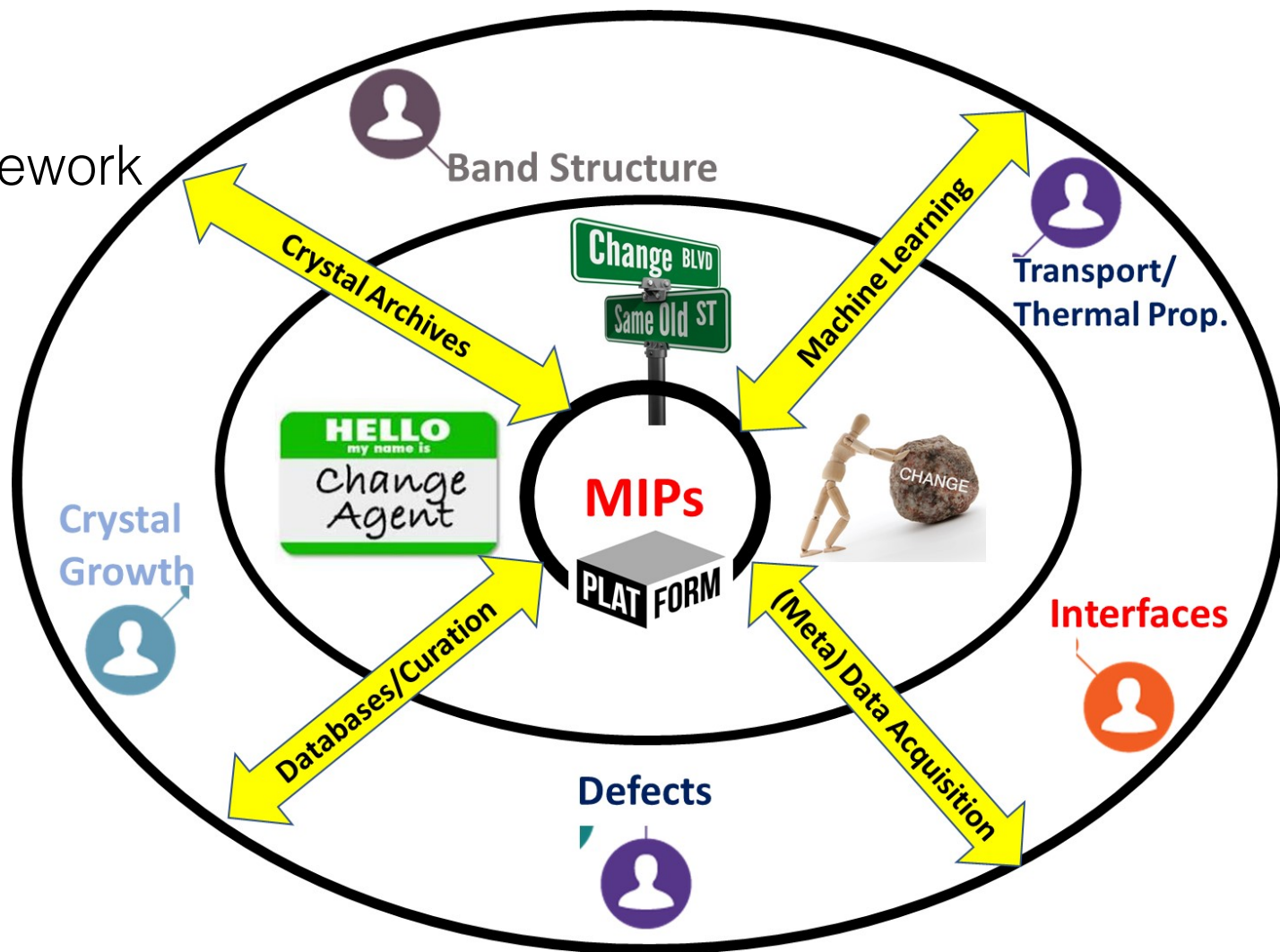
147 Total Attending
65 Poster presentations
41 Technical talks
4 guided discussions
1 network activity
2 interactive feedback sessions
1 Idea pit session
1 white paper 2D data pitch session



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NSF-2D Data Framework



20 awards (out of 31 submissions) will be made in the amount of \$2.5 M



upcoming data-related events

- Kick off-Student Training-2D Data Framework: materials data-centric training November 11-15 at Johns Hopkins in Baltimore, MD. This workshop is targeted for students and postdocs. Details about the workshop organized by the PARADIM MIP and Office of Data Informatics-NIST are available at: https://paradim.org/events/NSF_DMR_2018.
- Kick off-PI Meeting 2D Data Framework: MRS-Boston, MA.
- 2nd PI meeting Meeting 2D Data Framework: MRS Spring 2019.

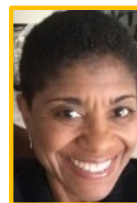


New members of the DMR-Data Working Group

- DMR-2D Data Framework-workshop organization, etc.
- Generate an understanding of ongoing investments at center level- what is missing?
 - Feed from prior reports- and open feedback- launch query to the community-
- PI White paper?

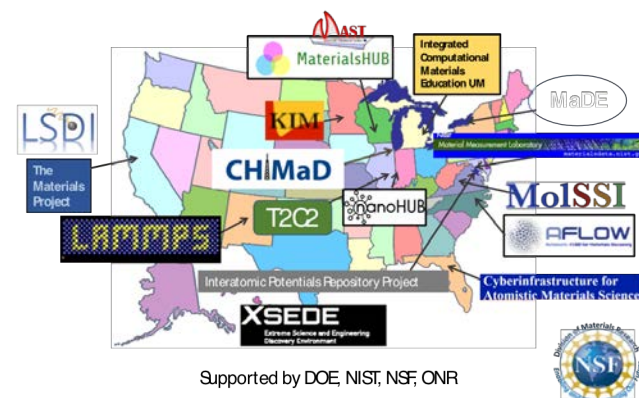


Lisa Lewis, Albion College

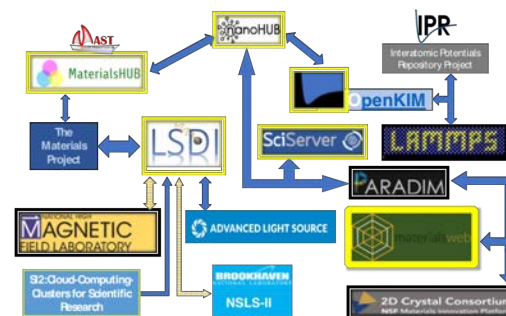


Claudia Johnson, Contractor

Materials Research Cyberinfrastructure

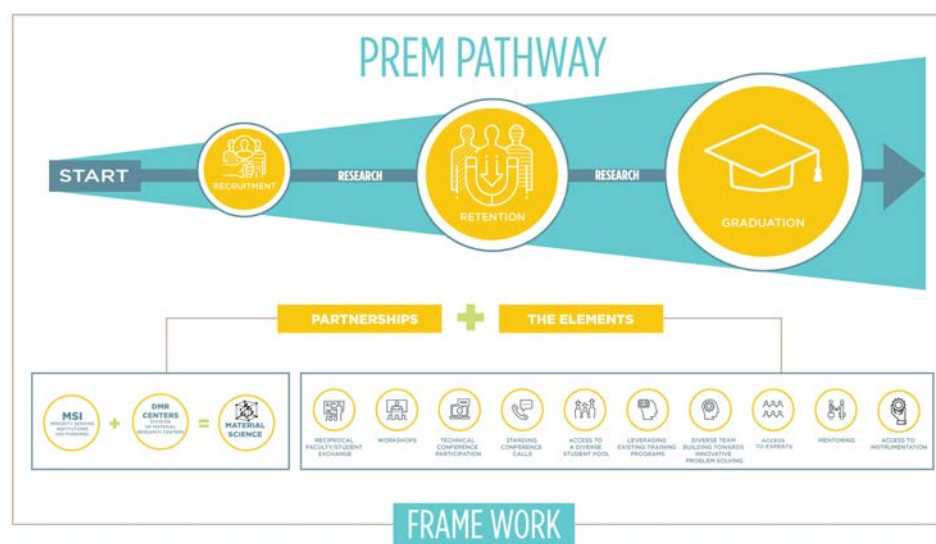


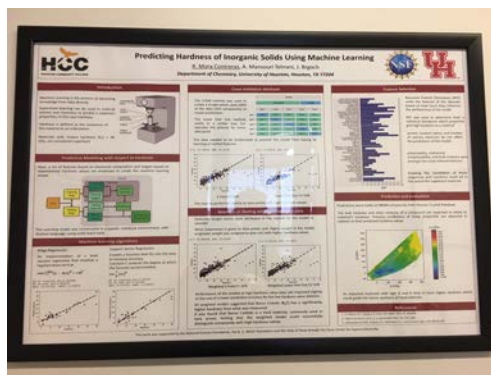
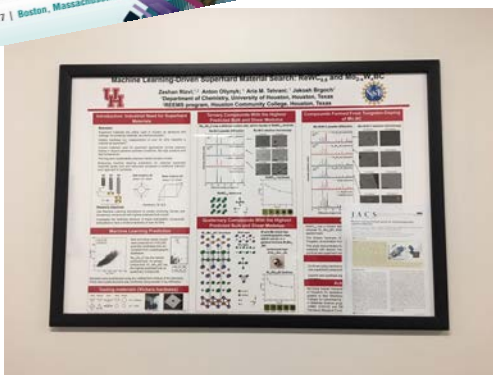
Part of a Materials Research Data-Resource Network



Solicitation 17-599

The PREM framework provides opportunities to all participants to contribute to some/all components of the PREM Pathway, focusing on different elements according to their research capacities.





Resource-leveraging is conducive to promoting diversity in data



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**PARTNERSHIPS BETWEEN
SCIENCE AND ENGINEERING
FIELDS AND THE NSF TRIPODS
INSTITUTES
(TRIPODS+X)**

WEBINAR: March 20, 2018

[https://www.nsf.gov/funding/pgm_summ.jsp?pi
ms_id=505527](https://www.nsf.gov/funding/pgm_summ.jsp?pi
ms_id=505527)



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<https://www.nsf.gov/attachments/244739/public/TripodsPlusXWebinar-Final.pdf>

TRIPODS GOAL

Transdisciplinary Research In Principles Of Data Science (TRIPODS) aims to bring together communities from **statistics, mathematics, and theoretical computer science** to develop the **theoretical foundations of data science** through institutes for **integrated research and training activities**.



TRIPODS + X

- Expands scope beyond data science foundations engaging researchers across other disciplines
- **Data-driven research and education challenges motivated by applications**
- Other activities aimed at building robust data science communities



Dear Colleague Letter: Advancing Long-term Reuse of Scientific Data

- Through this Dear Colleague Letter (DCL), the National Science Foundation's (NSF) Office of Advanced Cyberinfrastructure (OAC) announces its intention to support initial exploratory activities toward the creation of social and technical infrastructure solutions that further NSF's commitment to public access.

- **Community track**
- **Data reuse track.**
- **Socio-Technical Infrastructure**



The deadline for submission of Conference and EAGER proposals proposal submission date was May 23, 2018.

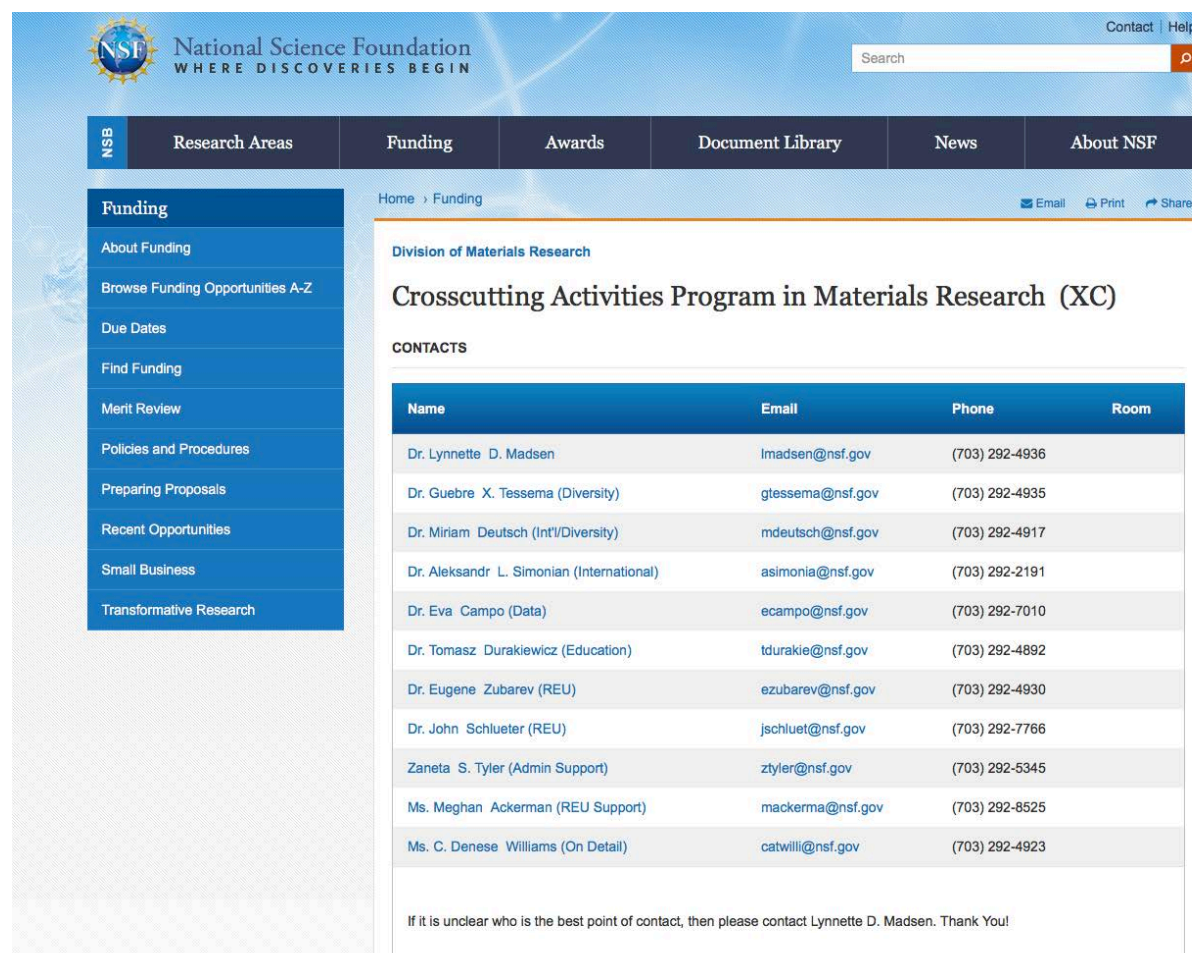
Data in X-Cutting Data Visualization Workshop

Workshop on the Convergence of Materials Research and Multi-Sensory Data Science

J. Rickman, Lehigh University

June 11-13, 2018

The creation of large data sets in all fields of endeavor is transforming the way work is done in the 21st century by providing opportunities to identify complex patterns and extract information that will enable new discoveries and expose pathways for advancing workplace efficiency. Unlocking the potential of large data to transform how people perform their jobs in areas as diverse as basic science, healthcare delivery and online marketing requires a convergence of data scientists, computer scientists and behavioral and cognitive scientists working alongside the experts in the field where workplace advancements will be made.



The screenshot shows the NSF Division of Materials Research website. The header includes the NSF logo, the text "National Science Foundation WHERE DISCOVERIES BEGIN", a search bar, and links for "Contact" and "Help". The navigation bar includes "Research Areas", "Funding", "Awards", "Document Library", "News", and "About NSF". The left sidebar lists various funding-related links. The main content area is titled "Division of Materials Research" and "Crosscutting Activities Program in Materials Research (XC)". Below this is a "CONTACTS" section with a table listing staff members, their email addresses, and phone numbers.

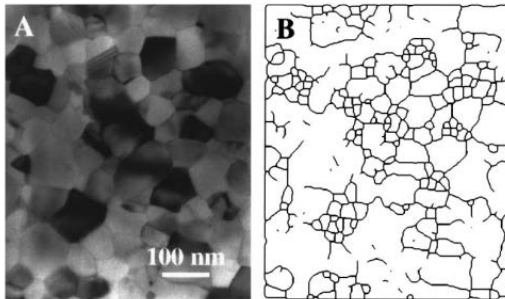
Name	Email	Phone	Room
Dr. Lynnette D. Madsen	lmadsen@nsf.gov	(703) 292-4936	
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Dr. Miriam Deutsch (Int'l/Diversity)	mdeutsch@nsf.gov	(703) 292-4917	
Dr. Aleksandr L. Simonian (International)	asimonia@nsf.gov	(703) 292-2191	
Dr. Eva Campo (Data)	ecampo@nsf.gov	(703) 292-7010	
Dr. Tomasz Durakiewicz (Education)	tdurakie@nsf.gov	(703) 292-4892	
Dr. Eugene Zubarev (REU)	ezubarev@nsf.gov	(703) 292-4930	
Dr. John Schlueter (REU)	jschluet@nsf.gov	(703) 292-7766	
Zaneta S. Tyler (Admin Support)	ztyler@nsf.gov	(703) 292-5345	
Ms. Meghan Ackerman (REU Support)	mackerma@nsf.gov	(703) 292-8525	
Ms. C. Denese Williams (On Detail)	catwilli@nsf.gov	(703) 292-4923	

If it is unclear who is the best point of contact, then please contact Lynnette D. Madsen. Thank You!



The promise of data science in microstructural recognition

TEM Image Processing

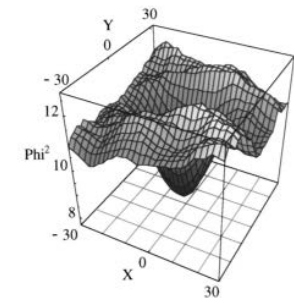
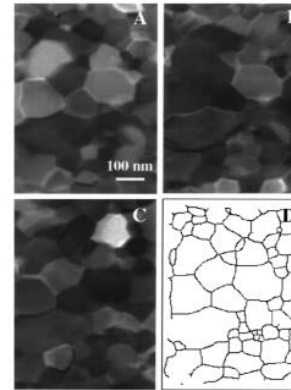


Typical bright-field TEM micrograph of a 100 nm Al film showing contrast ambiguities.

Tools Used:

median filter
Sobel edge detection
manual thresholding
skeletonization
dilation
erosion
closing

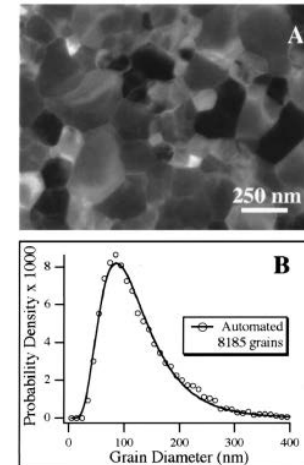
Improved Grain-Boundary Detection and Image Recombination



disregistry function for shifted micrographs

Grain-Size Distribution from Automated Analysis

- 8185 grains analyzed



$$p(x) = \frac{1}{\beta x \sqrt{2\pi}} \exp\left(-\frac{(\ln x - \alpha)^2}{2\beta^2}\right)$$

log-normal distribution

- **Role of Cognitive Science**

- Greater recognition of cognitive demands of data-intensive tasks.
- Better understanding of how humans interact with multi-dimensional data.

- **Education**

- Plans to incorporate data analytics into the materials curriculum.

Benefits of Convergence of Materials Science with Cognitive & Computer Science

- A new, powerful set of tools that supplements those in the materials toolbox.
- A greater appreciation of the role of cognitive processes in data interpretation.
- The development of a common language that mitigates interdisciplinary barriers.
- A better understanding of data curation issues that will dictate data availability and utility.



Dr. Alton Romig, Jr. delivers the plenary address.



Question on the table:
How can DMR help?

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