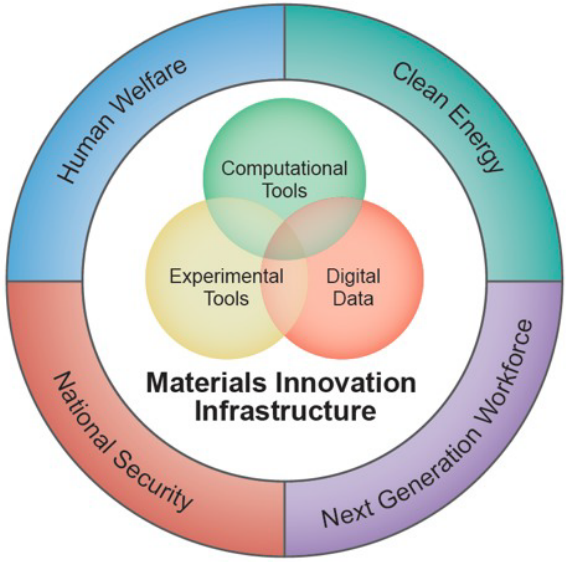
Multicomponent Diffusion Data and the Materials Genome

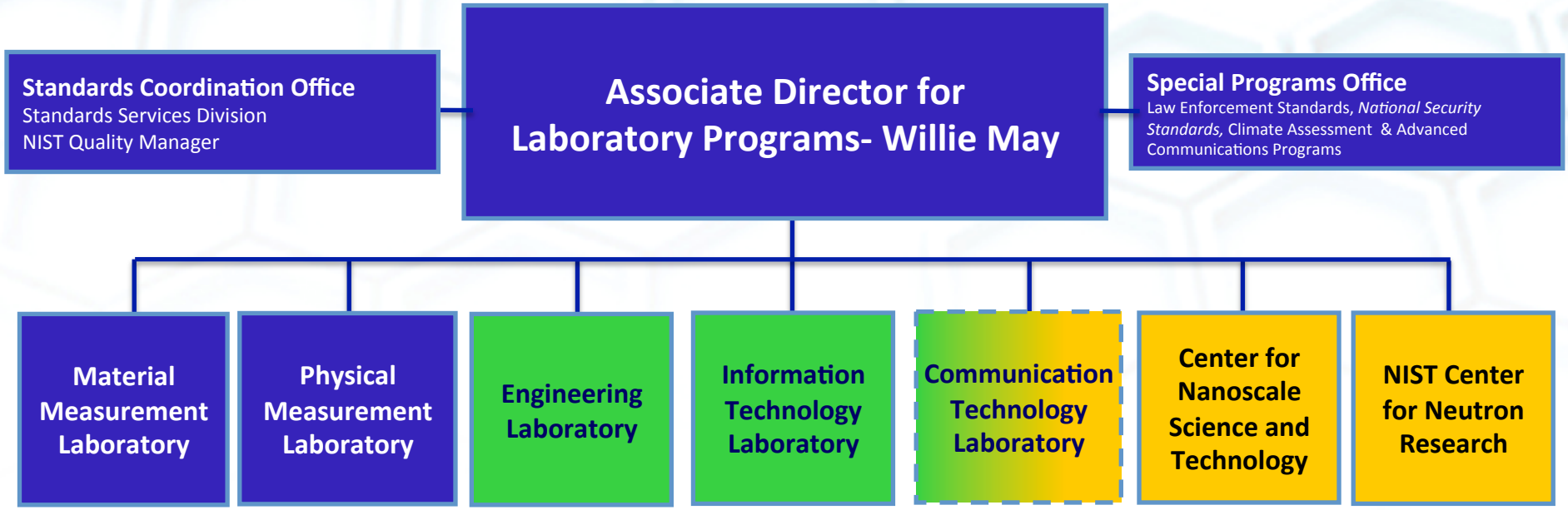
NIST Diffusion Workshop Series/CHiMaD CALPHAD Data

April 28-29, 2014

Sponsored by the Materials Science and Engineering Division



NIST LABORATORY PROGRAM

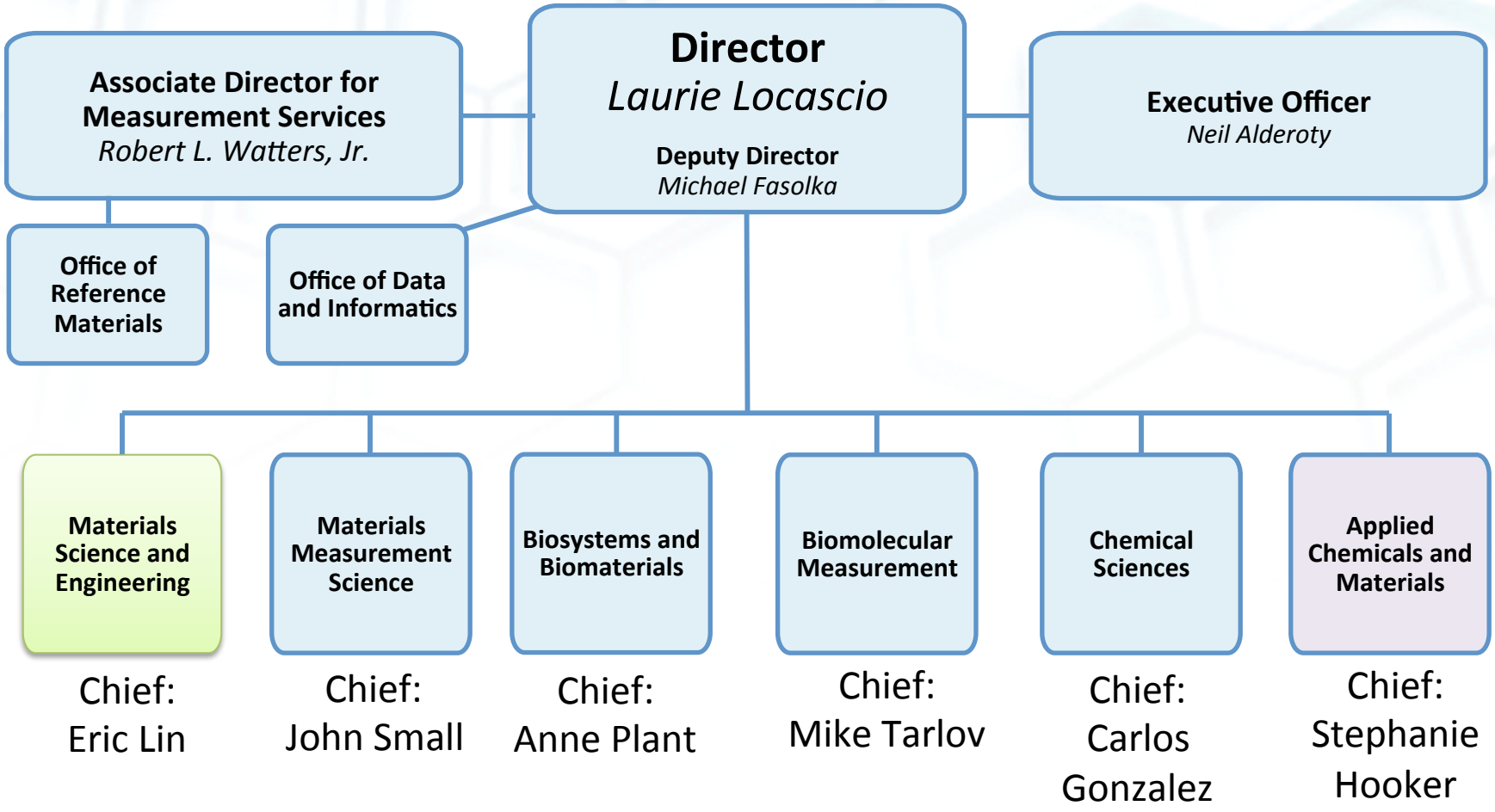


Metrology Laboratories	Technology Laboratories	National User Facilities
Driving innovation through Measurement Science and Standards	Accelerating the adoption and deployment of advanced technology solutions	Providing world class, unique, cutting-edge research facilities

NIST Lab Resources for FY13

- ~ $580 million from Direct Appropriations
- ~ $120 million from Other Federal and State Agencies
- ~ $50 million for other reimbursable services

Material Measurement Laboratory



MML AT A GLANCE

Locations

Gaithersburg, MD

Boulder, CO

Inst. for Bioscience and Biotech. Research (IBBR) University of Maryland

Hollings Marine Laboratory (HML) Charleston, SC

Brookhaven National Labs (BNL)
(NIST Beamlines at NSLS & NSLS-2)
Upton, NY

FY13 Fiscal Resources: ~ $150 M

- Direct Appropriation ~73%
- Other Government Agency ~ 16%
- Measurement Services ~ 11%

Staff:

~ 530 NIST Employees

~440 *Technical Staff*

~ 350 NIST Associates

NIST HISTORY: FACILITATING COMMERCE VIA MEASUREMENT SCIENCE & TECHNOLOGY

A world-leading measurement science and standards program

- Work resulting in 5 Nobel Prizes since 1997
- MacArthur Fellowship winner in 2003
- Kyoto Prize winner in 2011
- National Medal of Science winners in 1998 and 2008
- ~ 60 National Academy Members (10 current)
- ~120 National Society Fellows; recipients of ~ 60 National/International Awards per year

Bill Phillips
1997 Nobel Prize
in Physics

Eric Cornell
2001 Nobel Prize
in Physics

John Hall
2005 Nobel Prize
in Physics

Dan Shechtman
2011 Nobel Prize
in Chemistry

David Wineland
2012 Nobel Prize
in Physics

John Cahn
2011 Kyoto
Prize

- **Deep research expertise underpins technological innovation** – e.g., new materials, advanced clinical diagnostics and therapies, advanced communications, etc.
- **Non-regulatory status** enables important role as a convener that facilitates collaboration between industry and government

CENTER OF EXCELLENCE FOR ADVANCED MATERIALS RESEARCH

Center for Hierarchical Materials Design (CHiMaD)- led by Northwestern University

Consortium Members

- Northwestern-Argonne Institute of Science and Engineering
- Computation Institute (a partnership between the University of Chicago and Argonne)

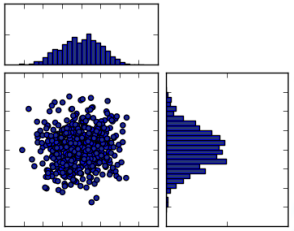
Others closely involved include

- QuesTek Innovations
- ASM International
- Fayetteville State University

Northwestern University
Evanston, IL

Focus: developing the next generation of computational tools, databases and experimental techniques to enable “Materials by Design”

Office of Data and Informatics



Key Functions

Next Generation of NIST SRD

- Strengthen marketing and distribution mechanisms
- Develop Quality Framework for reference data
- New Products and Delivery Modes: e.g. SRMDs

"Material" Data Science

- Data Mining and Analytics for Chem, Bio, Materials
- Knowledge Generation from Big Data in our Fields
- Metadata and interchange standards

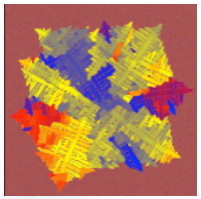
Resource for MML Researchers

- Best practices for Data Deluge
- Reduce Redundant Efforts
- Manage emerging trends in scholarly publishing

Liaison and Lead

- Key partners in ITL
- NIST/MML Efforts: MGI, Bioinformatics, Data Groups
- Government-wide directives/ interpret new regulations
- Champion data driven proposals

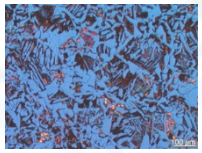
MATERIALS SCIENCE AND ENGINEERING



Chief: Eric Lin

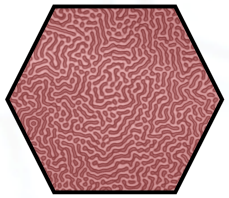
Division Function:

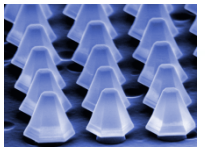
Provides the measurement science, standards, technology, and data required to support the Nation's need to design, develop, manufacture, and use materials.



Groups:

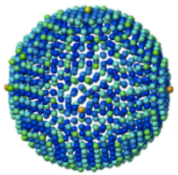
- Polymers & Complex Fluids (Kate Beers)
- Functional Polymers (Chris Soles)
- Functional Nanostructured Materials (Albert Davydov)
- Mechanical Performance (Jon Guyer)
- Thermodynamics and Kinetics (Carrie Campbell)





Capabilities:

- Metallurgical materials science (e.g. alloys, solidification, processing)
- Polymer & colloidal materials science (e.g. carbon nanotubes, nSoft)
- Microstructure, nanostructure (e.g. microscopy, scattering)
- Mechanical performance (NCAL, ballistic fibers)
- Materials data and computational tools (MGI)

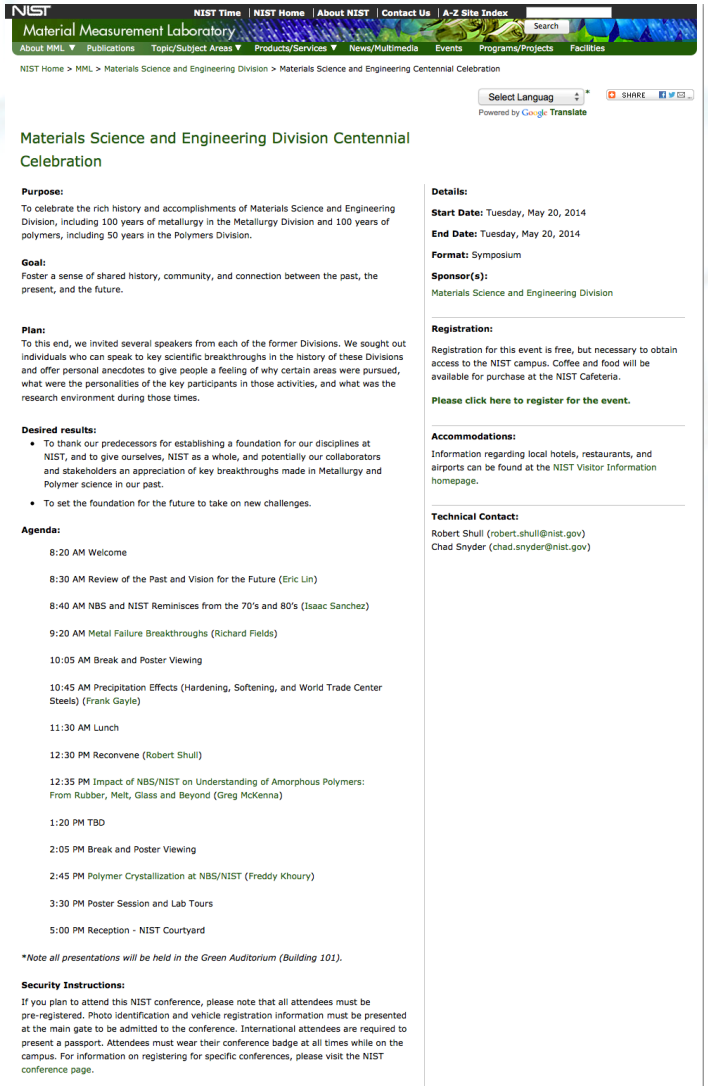


MATERIAL SCIENCE AND ENGINEERING CELEBRATION

MAY 20 , 2014

100 years of Metallurgy
50 years of Polymers

http://www.nist.gov/mml/msed/msed-centennial.cfm



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Material Measurement Laboratory

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Materials Science and Engineering Division Centennial Celebration

Purpose:

To celebrate the rich history and accomplishments of Materials Science and Engineering Division, including 100 years of metallurgy in the Metallurgy Division and 100 years of polymers, including 50 years in the Polymers Division.

Goal:

Foster a sense of shared history, community, and connection between the past, the present, and the future.

Plan:

To this end, we invited several speakers from each of the former Divisions. We sought out individuals who can speak to key scientific breakthroughs in the history of these Divisions and offer personal anecdotes to give people a feeling of why certain areas were pursued, what were the personalities of the key participants in those activities, and what was the research environment during those times.

Desired results:

- To thank our predecessors for establishing a foundation for our disciplines at NIST, and to give ourselves, NIST as a whole, and potentially our collaborators and stakeholders an appreciation of key breakthroughs made in Metallurgy and Polymer science in our past.
- To set the foundation for the future to take on new challenges.

Agenda:

8:20 AM Welcome

8:30 AM Review of the Past and Vision for the Future (Eric Lin)

8:40 AM NBS and NIST Reminisces from the 70's and 80's (Isaac Sanchez)

9:20 AM Metal Failure Breakthroughs (Richard Fields)

10:05 AM Break and Poster Viewing

10:45 AM Precipitation Effects (Hardening, Softening, and World Trade Center Steels) (Frank Gayle)

11:30 AM Lunch

12:30 PM Reconvene (Robert Shull)

12:35 PM Impact of NBS/NIST on Understanding of Amorphous Polymers: From Rubber, Melt, Glass and Beyond (Greg McKenna)

1:20 PM TBD

2:05 PM Break and Poster Viewing

2:45 PM Polymer Crystallization at NBS/NIST (Freddy Khoury)

3:30 PM Poster Session and Lab Tours

5:00 PM Reception - NIST Courtyard

**Note all presentations will be held in the Green Auditorium (Building 101).*

Security Instructions:

If you plan to attend this NIST conference, please note that all attendees must be pre-registered. Photo identification and vehicle registration information must be presented at the main gate to be admitted to the conference. International attendees are required to present a passport. Attendees must wear their conference badge at all times while on the campus. For information on registering for specific conferences, please visit the NIST conference page.

Details:

Start Date: Tuesday, May 20, 2014

End Date: Tuesday, May 20, 2014

Format: Symposium

Sponsor(s):

Materials Science and Engineering Division

Registration:

Registration for this event is free, but necessary to obtain access to the NIST campus. Coffee and food will be available for purchase at the NIST Cafeteria.

Please click here to register for the event.

Accommodations:

Information regarding local hotels, restaurants, and airports can be found at the NIST Visitor Information homepage.

Technical Contact:

Robert Shull (robert.shull@nist.gov)
Chad Snyder (chad.snyder@nist.gov)

Agenda

Tuesday, April 29
NIST Diffusion Workshop /CALPHAD Proto Data Workshop (Joint Session)

8:30-9:00 Introduction and Welcome to NIST

9:00-9:30 "Essential information to build up the diffusion genome," John Ågren (KTH)

9:30-9:45 Discussion

9:45-10:30 Update on NIST Materials Data Informatics Efforts (Campbell, Kattner, Dima, Youssef, Bartolo)

10:30-11:15 "Augmenting NIST/TRC Data Technologies to Aid the Materials Community" (Kenneth Kroenlein and Vladimir Diky, Thermodynamic Research Center, NIST)

11:15-11:30 Data and Simulation Management Tools (Dan Wheeler, NIST)

11:30-12:00 Discussion/Diffusion Workshop Wrap-up

Agenda

Wednesday April 30

8:45-9:00 Logistics

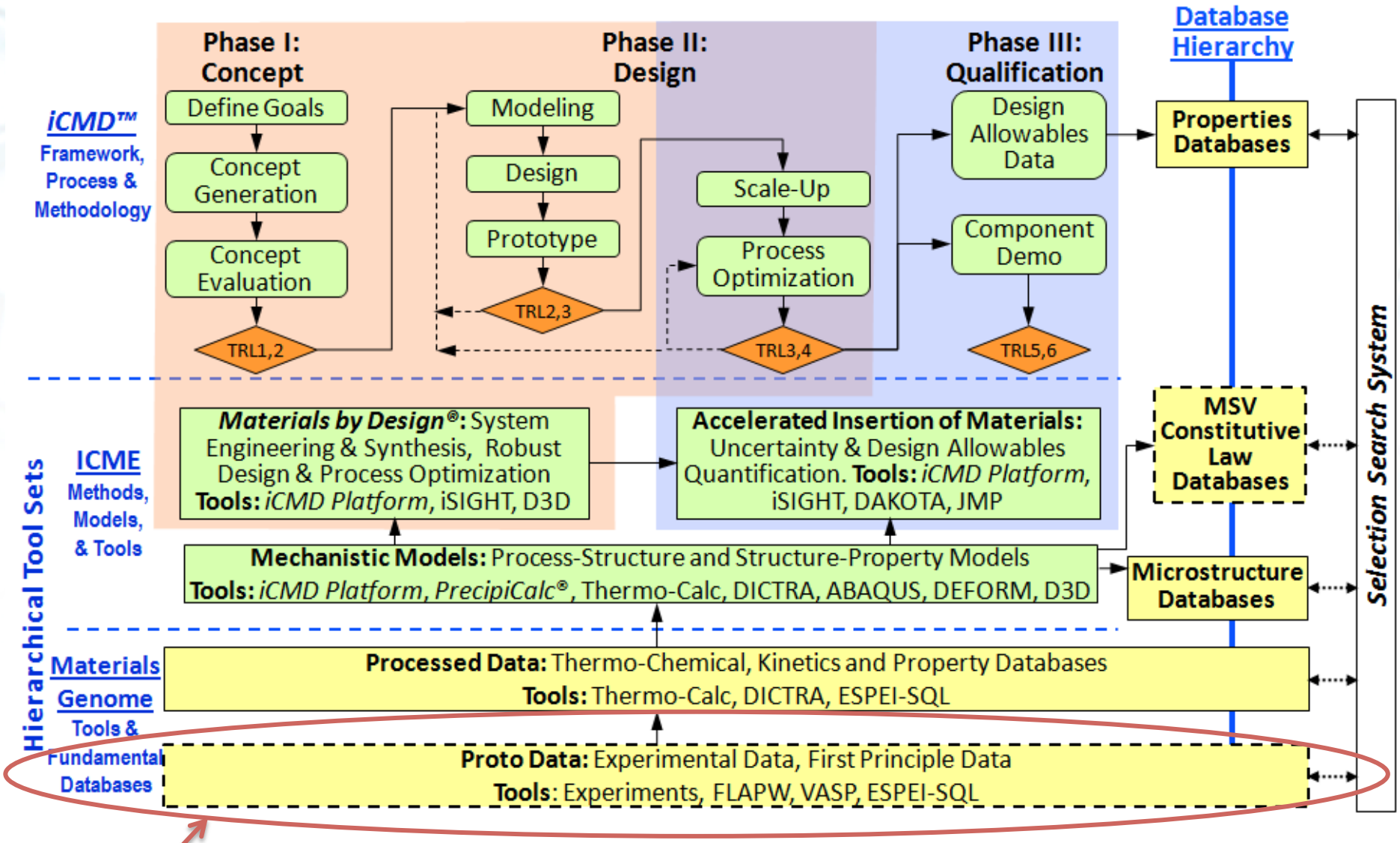
9:00-9:30 Data Federation Discussion, Laura Bartolo (Kent State)

9:30-10:00 Discussion on Community Involvement and Support (Interactions with Publishers)

10:00-10:15 Break

10:15-11:00 Ontology Building: Term Association

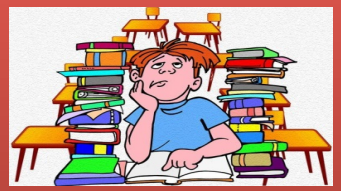
11:00-11:30 Workshop wrap-up: How to keep the process moving forward



Focus for workshop (phase-based property data needed to build Composition, temperature, pressure dependent CALPHAD-base databases

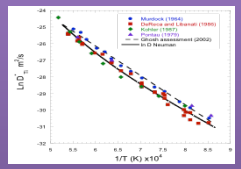
G. B. Olson, 2013

Current Assessment Process

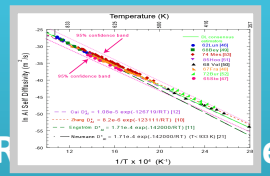


Search data

Digitize Data



Plot data



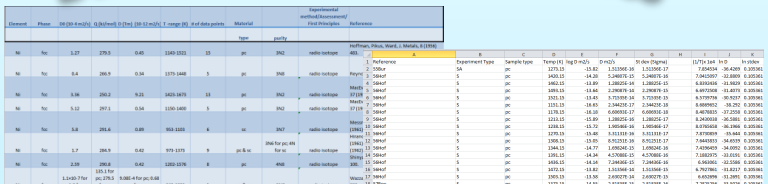
for Assessment use

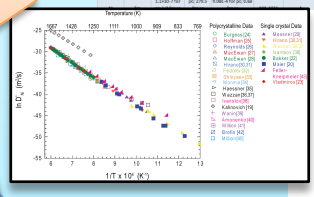
Future

Search infrastructure

CALPHAD user needs data for A-B-C system,

Computational and Experimental Databases and Repositories





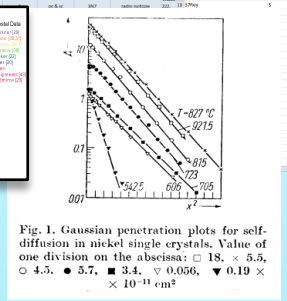


Fig. 1. Gaussian penetration plots for self-diffusion in nickel single crystals. Value of one division on the abscissa: □ 18, × 5.5, ○ 4.5, ● 5.7, ■ 3.4, ▽ 0.056, ▼ 0.19 × × 10^{-11} cm²

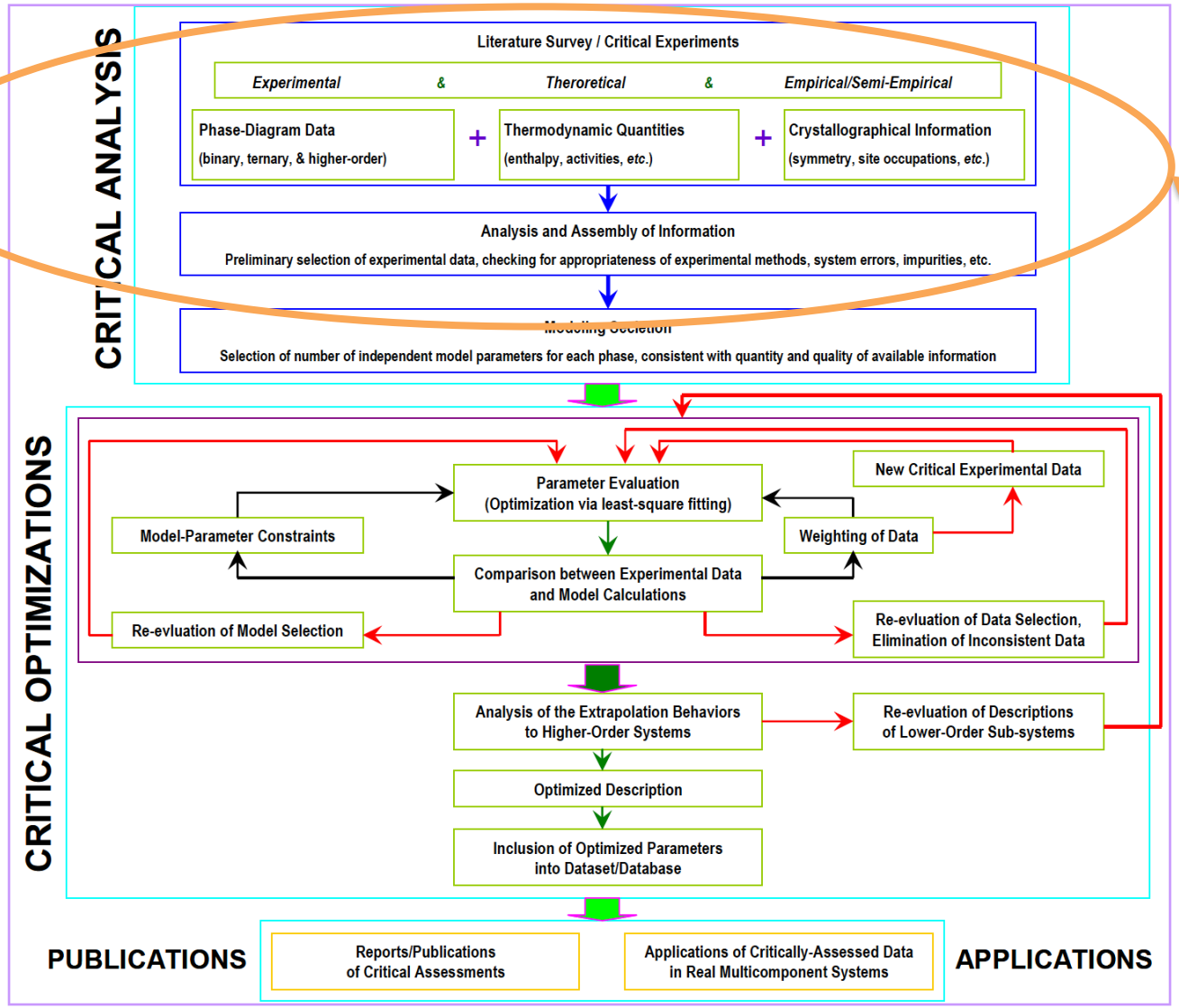
Federated System

Interfaces for input of computational and experiment data

Search returns available data And points out missing data

PURPOSE OF A PHASE BASED DATA REPOSITORY SYSTEM:

FACILITATE CRITICAL ANALYSIS PART OF THE ASSESSMENT PROCESS.
WILL NOT REPLACE ASSESSOR'S JUDGMENT ON MODEL SELECTION OR WEIGHTING OF DATA



Data repository would make this part of the process more efficient

Thermo-Calc User's Manuel: Version S p 12-4

Agenda

Monday, April 28

8:30-9:00 Introductions and Welcome (Coffee and Bagels will be available)

9:00 -9:30 “Short-Circuit Diffusion In Recrystallizing Microstructure: Diffusion Properties of a Recrystallization Front,” Sergiy Divinski (University of Münster)

9:30-10:00 “Design and Modeling of Grain Boundary Diffusion Experiments in Magnesium Thin Films using SIMS,” Nagraj Kulkarni

10:00-10:30 Discussion/Break

10:30-11:00 “Chemical Diffusivities and their Hidden Concentration Units,” John Morral (Ohio State University

11:00-11:30 “Precipitation simulation of Ni-base superalloys, Fan Zhang (CompuTherm)

11:30-11:45 Discussion

11:45-1:00 Lunch (NIST Cafeteria)

Agenda

Monday, April 28

1:00-1:30 "Diffusion and Mobility in Co-Al-based Ternary Alloys: Diffusion Couple Experiment and Assessment," Yuwen Cui (IMDEA Materials Institute)

1:30-2:00 "Diffusion in Co-Al-W-Ni System: Initial Diffusion Couple Observations," Kil-Won Moon, Eric Lass, Carrie Campbell, William Boettinger (NIST)

2:00-2:30 "Mobility Database Development for Magnesium Alloys," Michele Manuel, (University Florida)

2:30-3:00 "Role of Solid State Diffusion Studies in Materials Selection and Process Design for Development of Low Enrichment U-Mo Metallic Nuclear Fuel Systems," Yongho Sohn (University of Central Florida)

3:00-3:30 Discussion/Break

3:30-4:00 "Automating ab initio diffusion calculations with the MAterials Simulation Toolkit (MAST)" Dane Morgan, (University of Wisconsin)

4:00-4:30 "Ti-O-M interaction between oxygen and metal (M) substitution in titanium for oxygen diffusion change," Dallas Trinkle (University of Illinois)

4:30-5:00 "Diffusion of Oxygen in Ni and Fe due to Substitutional Vacancy from DFT calculations," Zi-Kui Liu (Penn State University)

5:00-5:30 Discussion

6:00 Workshop dinner