IG RDA/CODATA Materials Data, Infrastructure, & Interoperability (MDII) Sessions 1 & 2

WEDNESDAY, 26/3, 1330-1500 & 1530-1700

CO-CHAIRS

JIM WARREN, NIST

LAURA BARTOLO, KSU

SUMMARY SESSIONS 1 & 2

Purpose of IG:

To overcome challenges and realise opportunities in the development of the global *materials* innovation infrastructure based on interoperability and open standards for the management, exchange, and analysis of *materials* data (models too)

Focus of P3 IG MDII two sessions:

Highlight some current materials data issues & projects

Identify IGs & WGs with complementary interests

Aspirational Deliverables/Goals for Sessions 1 & 2:

- Easy: Connect with related IGs & WGs
- Easy: Explore opportunities for outreach
- Medium: Develop joint use cases
- Hard?: Set up one Working Group

To help businesses discover, develop, and deploy new materials twice as fast, we're launching what we call ***the Materials Genome Initiative****. The invention of silicon circuits and lithium ion batteries made computers and iPods and iPads possible, but it took years to get those technologies from the drawing board to the market place. We can do it faster.*

-President Obama
Carnegie Mellon University, June 2011

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The Materials Genome Initiative

Goal: to decrease the cost and time-to-market by 50%

1. Develop a Materials Innovation Infrastructure

2. Achieve National goals in energy, security, and human welfare with advanced materials

3. Equip the next generation materials workforce

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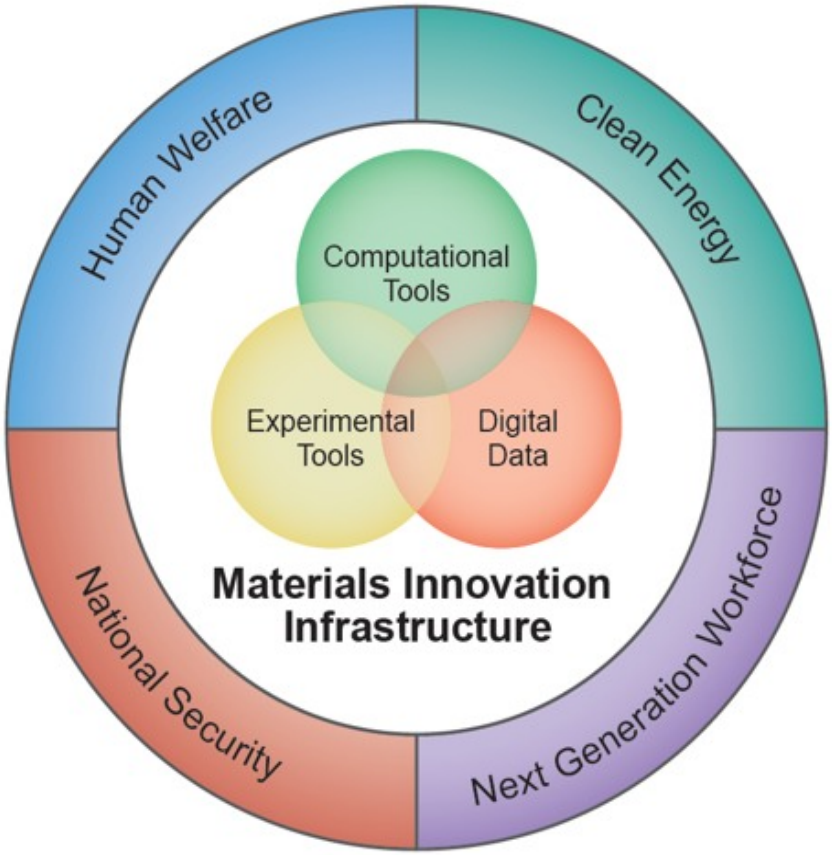
The Materials Innovation Infrastructure

Three-pronged approach to advance materials design



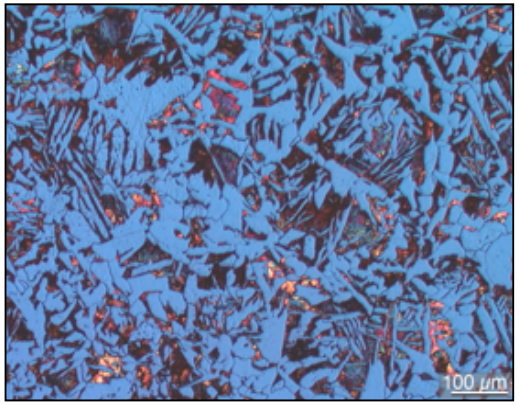
"The Materials Genome Initiative will develop new integrated computational, experimental, and data informatics tools. These software and integration tools will span the entire materials continuum, be developed using an open platform, improve best-in-class predictive capabilities, and adhere to newly created standards for quick integration of digital information across the materials innovation infrastructure."

Why a Materials Genome Initiative?

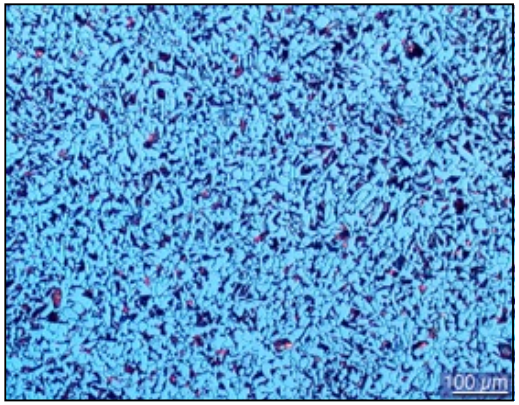
Materials Are Complicated Systems
Modeling is a Challenge

- Advanced materials are complex: multi-component and multi-phase
- Without adequate modeling, informatics and data exchange, the development of next generation materials using empirical approaches is bogged down by their complexity
- The Materials Genome Initiative seeks to advance materials design capabilities to promote faster, cheaper

Alloy cooled from 300 °C



Alloy cooled from 800 °C



- Composition and processing affect properties
- Phases change as a function of processing
- Microstructures consist of mixtures of multiple material phases
- Finer microstructure results in a much stronger alloy

NIST
National Institute of Standards and Technology
U.S. Department of Commerce

SESSION 1

1330 – 1500

Session Start

Around the table introductions

CODATA & Preamble, Laura Bartolo, KSU, Co-Chair

Materials data issues and approaches presentations:

- ICME Data Formats, e.g. MatML, Scott Henry, ASM
- ICMEg, Georg Schmitz, RWTH Aachen University
- Phase based property data & other NIST efforts, Jim Warren, NIST
- SERES, Tim Austin, European Commission Joint Research Centre
- DataNet Federation Consortium, Bill Regli, Drexel University

Representatives from other IGs & WGs

- IG Big DATA Analytics, Morris Riedel, Juelich Supercomputing

Discussion of presentations & review of upcoming session

BREAK 1500 – 1530

CODATA ORGANIZATIONAL STRUCTURE: OVERVIEW, TASK GROUP & COLLABORATION

Overview

Committee on Data for Science & Technology, 1966, ICSU affiliation

US CODATA is located within the National Academy of Sciences

- → **Non-governmental, international (int'l), interdisciplinary**
- → **Improve scientific & technical data management & use**
- → **22 national members with its work done by int'l task groups**

Materials TG

Exchangeable Mat'ls Data Representation to support Scientific Research and Education

- → **8 countries with representation across Europe, North America, and the Pacific**
- → **Good representation in national data centers, government labs & universities**
- → **CODATA has long history and interest in materials science & engineering**

Collaboration

RDA & CODATA bring together different constituents who share common interest

- → **RDA brings technical focus though not its only focus**
- → **CODATA brings data policy focus though not its only focus**
- → **Sponsor joint workshops and meetings to increase progress**

RDA/CODATA IG MDII: PREAMBLE

- **Scientific endeavor rests on free and open exchange of ideas and supporting data**

- **Sharing computational & experimental materials data through online repositories, standardized formats & terminologies, and open programming interfaces is essential to accelerate advance materials discovery, design, & development.**

- **Free & widely available data creates increased opportunities for conducting fundamental research while facilitating potential commercial data services.**

- **Scientific & economic interest of all countries gain under a framework of free & open data exchange where intellectual property & national security are respected.**

SESSION 1 PRESENTATIONS

Materials data issues and approaches presentations:

- **ICME Data Formats, e.g. MatML, Scott Henry, ASM**
- **ICMEg, Georg Schmitz, RWTH Aachen University**
- **Phase based property data & other NIST efforts, Jim Warren, NIST**
- **SERES, Tim Austin, European Commission Joint Research Centre**
- **DataNet Federation Consortium, Bill Regli, Drexel University**

Representatives from other IGs & WGs:

- **IG Big DATA Analytics, Morris Riedel, Juelich Supercomputing**

SESSION 2

1550 – 1700

Review Session 1, Laura Bartolo, KSU, Co-Chair

Around the table introductions of new participants

Representatives from other IGs & WGs

WG Data Type Registry, Larry Lannom, CNRI

RDA-CODATA IG Legal Interoperability, Paul Uhlir, NAS

Aspirational Deliverables/Goals, Jim Warren, NIST, Co-Chair

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Wrap-up