CHiMaD Data Schema Working Group

Report
Topics of Today's Discussion

• Thermomechanical Processing History
• Hardness Testing
• Nanomine
• CALPHAD Protodata
• Workflow tool integration
• NoMaD Repository
• ASM Taxonomy
Goals of 3 Month Project

- Identify dataset(s) for curation in MDCS
- Discuss and agree on shared terminology for
  - metadata (e.g., strain rate)
  - data (e.g., load vs. displacement)
  - derived data (e.g., modulus of elasticity)
- Create reusable XML schema types
- Create scripts for data transformation
- Curate dataset(s) in MDCS
Materials Data

- Discoverable
- Accessible
- Interoperable

- Discoverable
- Accessible
- Maybe Not Interoperable

- Not Discoverable
- Not Accessible
- Maybe Not Interoperable

Nat Neurosci, 17(11), 1442-1447.
doi:10.1038/nn.383
Materials Data

The Materials Project
OQMD
https://materialsdata.nist.gov

Organized big data
Long-tail data

Literature limit

Unpublished and dark data

Data size

Nat Neurosci, 17(11), 1442-1447.
doi:10.1038/nn.383
A Configurable Data Curation System

Configurable Interface

Data Management & Search Engine

Structured Data

Large/Binary Files

Your Data Repository or Your Resource Registry
Long Tail

Nat Neurosci, 17(11), 1442-1447.
doi:10.1038/nn.383
NIST MGI APPROACH TO LONG TAIL DATA

- **Discoverable**
  (via the Registry)
  https://mgi.nist.gov/Zkp

- **Accessible**
  (via the Curator)
  https://mgi.nist.gov/ZkS

- **Interoperable**
  (via Community Data Standards)
  https://mgi.nist.gov/ZkG
Group Activities/Discussion
Draft Thermomechanical Processing History Schema
Draft Hardness Testing Schema
Statistical Learning and Analysis Module Tools

Statistical learning and analysis modules include web and downloadable packages that can be used to pre-process and analyze structure and material property data. Each of the modules will specify required format of input and output data, and provide a brief introduction of mechanism of the algorithm.

**NIBLACK BINARIZATION**

Descriptor Characterization is a modular tool that takes input from a micrograph image of a microstructure of material and generate statistical descriptors that can characterize the structure information. More details to follow.

**DESCRIPTOR CHARACTERIZATION**

Descriptor Characterization is a modular tool that takes input from a micrograph image of a microstructure of material and generate statistical descriptors that can
Nanomine

207 results

- L180_S6_Maillard_2012 polymer nanocomposite
  - PolymerNanocomposite
  - ID: L180_S6_Maillard_2012
  - DATA_SOURCE
    - Citation
  - MATERIALS
    - Polymer
    - Particle
  - PROCESSING
    - SolutionProcessing
  - CHARACTERIZATION
    - Transmission_Electron_Microscopy
    - Atomic_Force_Microscopy
  - PROPERTIES
    - Mechanical
      - Tensile
        - TensileModulus
        - ElongationAtBreak
    - L180_S5_Maillard_2012 polymer nanocomposite
    - L180_S4_Maillard_2012 polymer nanocomposite
    - L180_S3_Maillard_2012 polymer nanocomposite
    - L180_S2_Maillard_2012 polymer nanocomposite
    - L180_S1_Maillard_2012 polymer nanocomposite
**Curating Diffusion Data**

### Sample Information
- Sample Id,
- Owner
- Date of Experiment

### End Member Material Information
- Phase name
- Crystal structure
- Phase Fraction
- Composition
- Processing

### Experimental Procedures

### Diffusion Annealing Conditions

### Collected Data
- Spreadsheet
- Micrograph
CALPHAD Protodata

Self Diffusion Resource

http://www.ctcms.nist.gov/~gkl/selfdiffusion.html
## CALPHAD Protodata

<table>
<thead>
<tr>
<th>Method</th>
<th>Structure</th>
<th>Diffusion Direction</th>
<th>Frequency Factor D0 (m^2/s)</th>
<th>Activation Energy Q (kJ/mole)</th>
<th>Temperature (K)</th>
<th>Details</th>
<th>Reference</th>
<th>Raw data</th>
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**Method:** Experimental  
**Structure:** FCC  
**Direction:** Isotropic  
**Author:** Lundy  
**Year:** 1962  

\[
D = D_0 \exp\left(-\frac{Q}{RT}\right)  
\]

\[
* D = D_0^1 \exp\left(-\frac{Q_1}{RT}\right) + D_0^2 \exp\left(-\frac{Q_2}{RT}\right)  
\]

\[
** D = D_0 \exp\left(-\frac{Q}{RT}\right) \exp\left(\frac{\Omega(T_M)^2}{T^2}\right)  
\]
Workflow Tool Integration

Experimental Analysis Groups

- **NAIVE**: Proprietary Software e.g: TA SW v2.0
- **INTERMEDIATE**: Excel formulas and charts
- **EXPERT**: Python Scripting and Matlab

Difficulties in sharing
Workflow Tool Integration

Reproducibility: MS Galaxy workflow
Workflow Tool Integration

Capabilities for MS-Galaxy users

How different levels of user can take advantage of galaxy

**NAIVE**
- Store data and perform analysis

**INTERMEDIATE**
- Design workflows

**EXPERT**
- Create custom tools for MS galaxy
NoMaD Repository

NOMAD

Search by name or description
molec

Select Parent Section
Any Section

Select Abstract Type
Any Abstract Type

Select Type
Any Meta Info Type

section_run  section_sampling_method  settings_molecular_dynamics

settings_molecular_dynamics direct children:
settings_barostat
settings_integrator
settings_thermostat
NoMaD Repository
ASM Taxonomy

- metal
  - ferrous
  - nonferrous
  - aluminum
    - cast-aluminum
      - series-1xx.x-pure-aluminum
      - series-2xx.x-aluminum-copper
      - series-3xx.x-aluminum-silicon-plus-copper
      - series-4xx.x-aluminum-silicon
      - series-5xx.x-aluminum-magnesium
      - series-7xx.x-aluminum-zinc
      - series-8xx.x-aluminum-tin
      - series-9xx.x-aluminum-plus-other-elements
      - unclassified-cast-aluminum
    - wrought-aluminum
      - cobalt
      - copper
      - gold
Closing Remarks

• New Schemas

• Integration