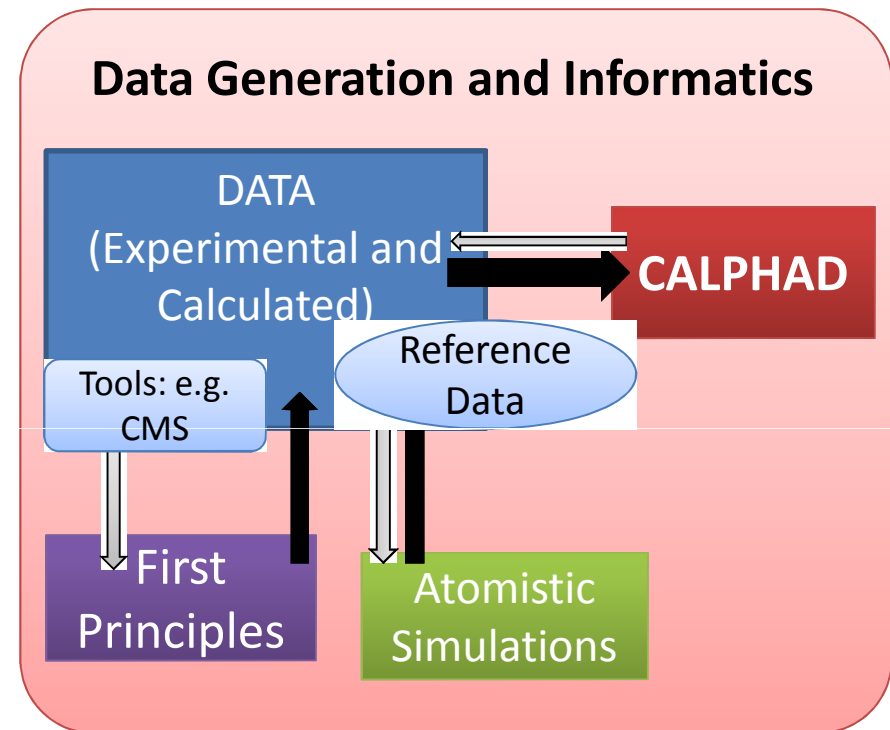
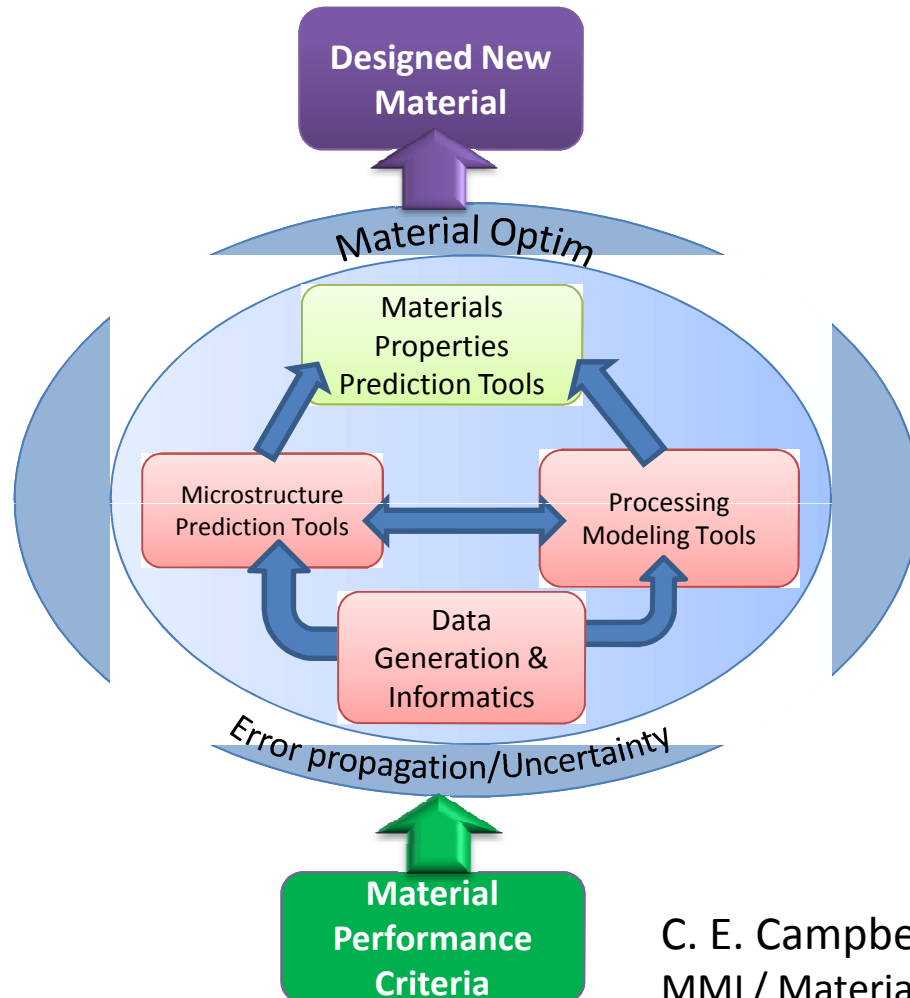


Materials Data and Informatics

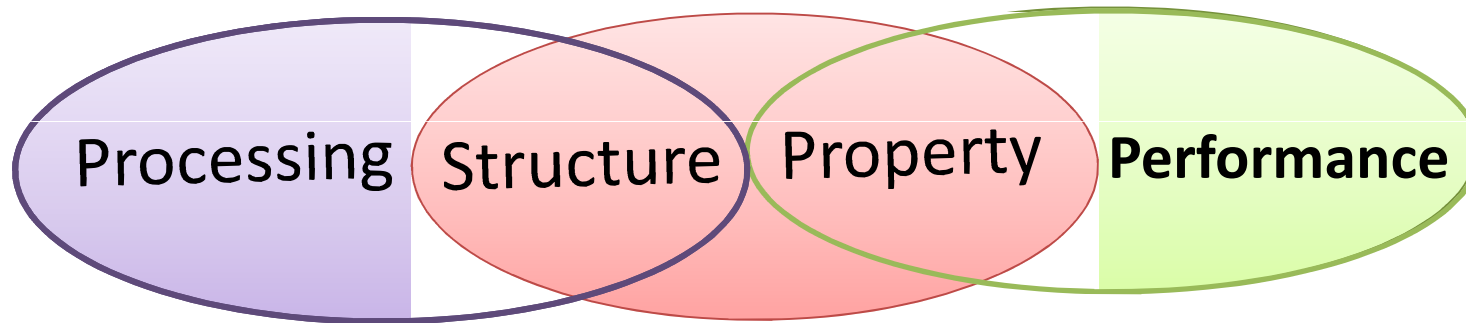


C. E. Campbell and A. Dima
MML/ Materials Science and Engineering Division and ITL/Software
and Systems Division

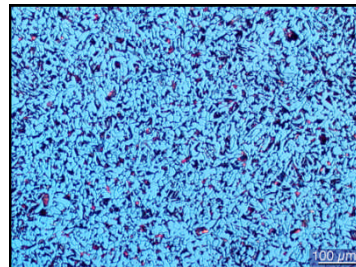
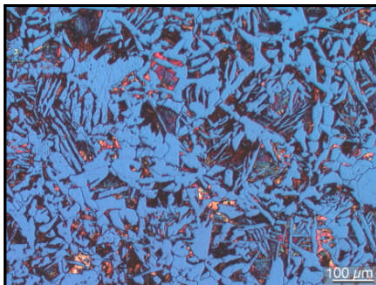
May 2nd, 2013

Materials Are Complicated Hierarchical Systems

- Advanced materials often consist of **several components** (generally, $n > 5$) and **multiple phases**.
- The material **properties are dependent on the microstructure**.
- **The microstructures changes as a function of processing and service conditions.**



Material A at Temp 1



Material A at Temp. 2

Key to material design:

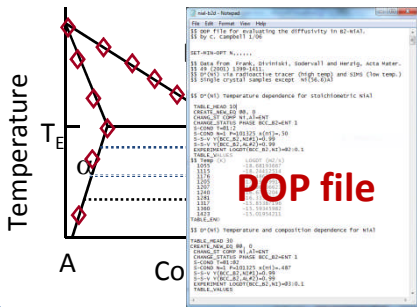
- What phases are present
- Composition and morphology of the phases present

 **CALPHAD**

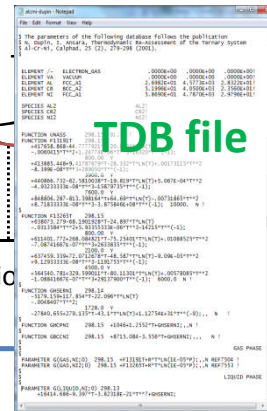
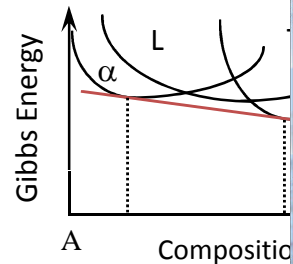
CALPHAD Approach

- Collected experimental and computational data are used to fit functions.
- Functions are used to calculate phase equilibria, including phase diagrams.

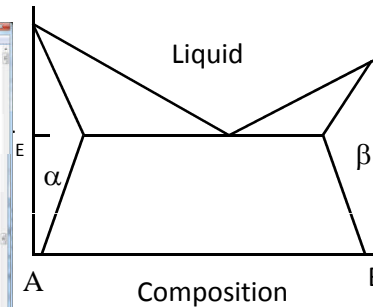
Experimental phase diagram and thermochemical data



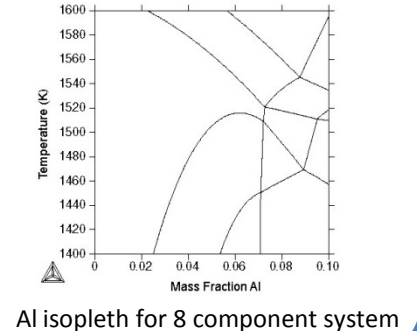
Determine Gibbs energy functions for each phase:
 $G = f(x, T, P)$



Calculated phase diagram



Combine binaries and ternaries to predict multi-component systems



$$G^{\phi} = G^0 + G^{ideal} + G^{excess}$$

Binaries ➡ Ternaries ➡ Quaternaries ➡ n^{th} Order Systems

➡ True quaternary compounds are rare in metallic systems

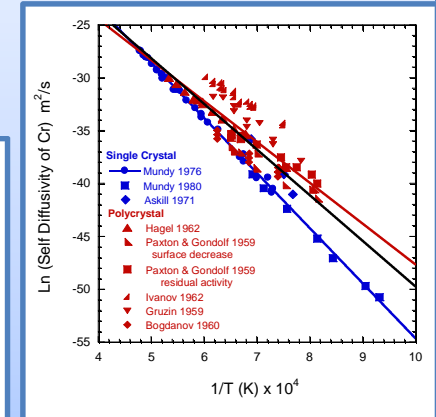
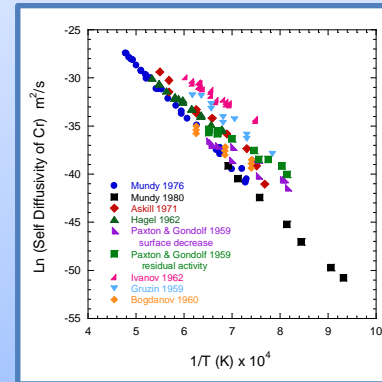
➡ Assessment of ternary systems is usually sufficient for the description of a multicomponent system

➡ Same methodology can be applied to the description of other property data

Informatics Challenges Associated with CALPHAD data

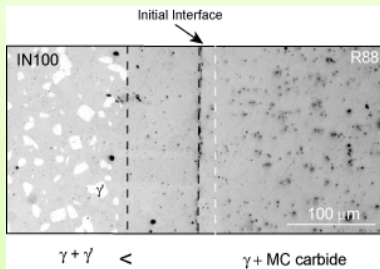
Need to classify and differentiate data

- Need to determine which data to evaluate
- Example: Cr Self-Diffusion Data
 - Separate single crystal from polycrystal data.
 - Only use single crystal data to determine reference values.
- Other examples of sorts include material purity, measurement technique, etc.,



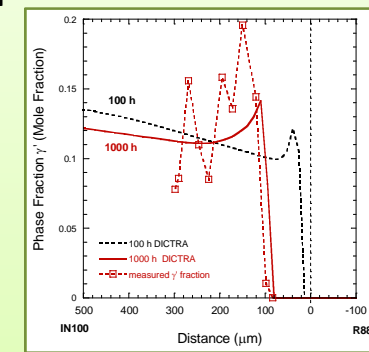
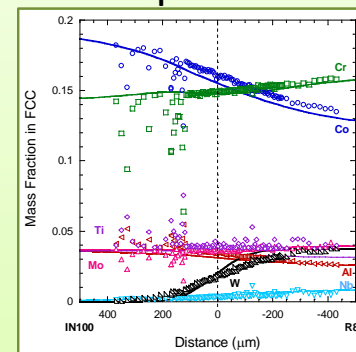
Does experiment = calculation?

Diffusion example: Does the simulation include all the phases in experiment?



IN100/René-88 at 1150 °C for 1000 h

If γ' and MC carbide not included, cannot predict the position of the $\gamma + \gamma' / \gamma + \text{MC}$ interface correctly



- Do the boundary conditions match the experimental geometry?
- Are the heating and cooling rates used in the experiment included in the calculation?

Examples of CALPHAD Data Types

For each assessment: Evaluated data file (e.g., POP, DOP)

Functional descriptions for phase quantity (e.g., TDB)

- Emphasis on binary and ternary data to predict multicomponent properties
- Data can be experimental or computational.

1-D (Points)

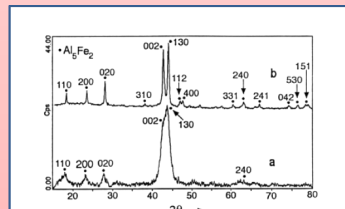
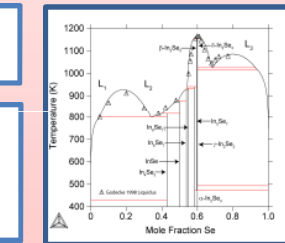
Melting Temperatures

Critical Temperatures
(Phase Changes)

Lattice Parameters

Heat of Formations

Phase Fractions
and Compositions



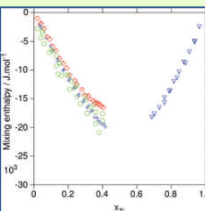
Tracer
Diffusivities

Activation Energies

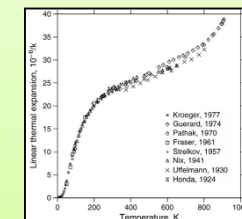
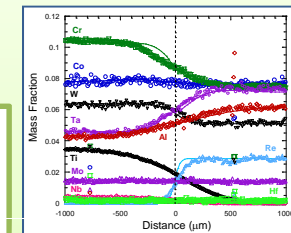
2-D (Lines)

Composition
Profiles

Heat Capacities



Enthalpies of Mixing

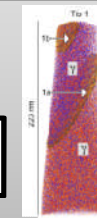
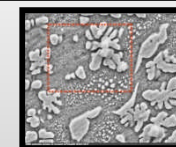
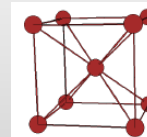


3-D

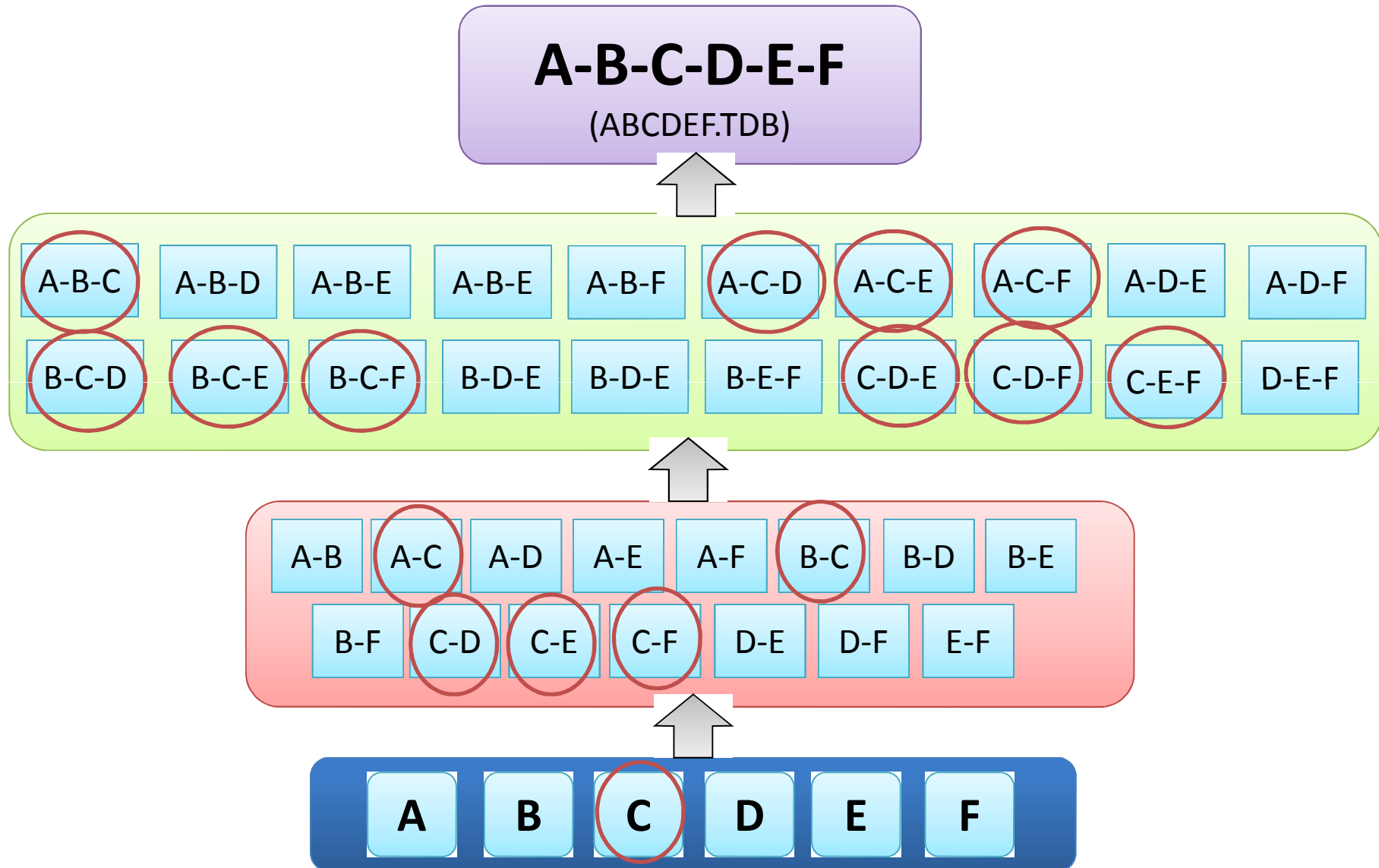
Crystal Structures

Micrographs/Morphologies

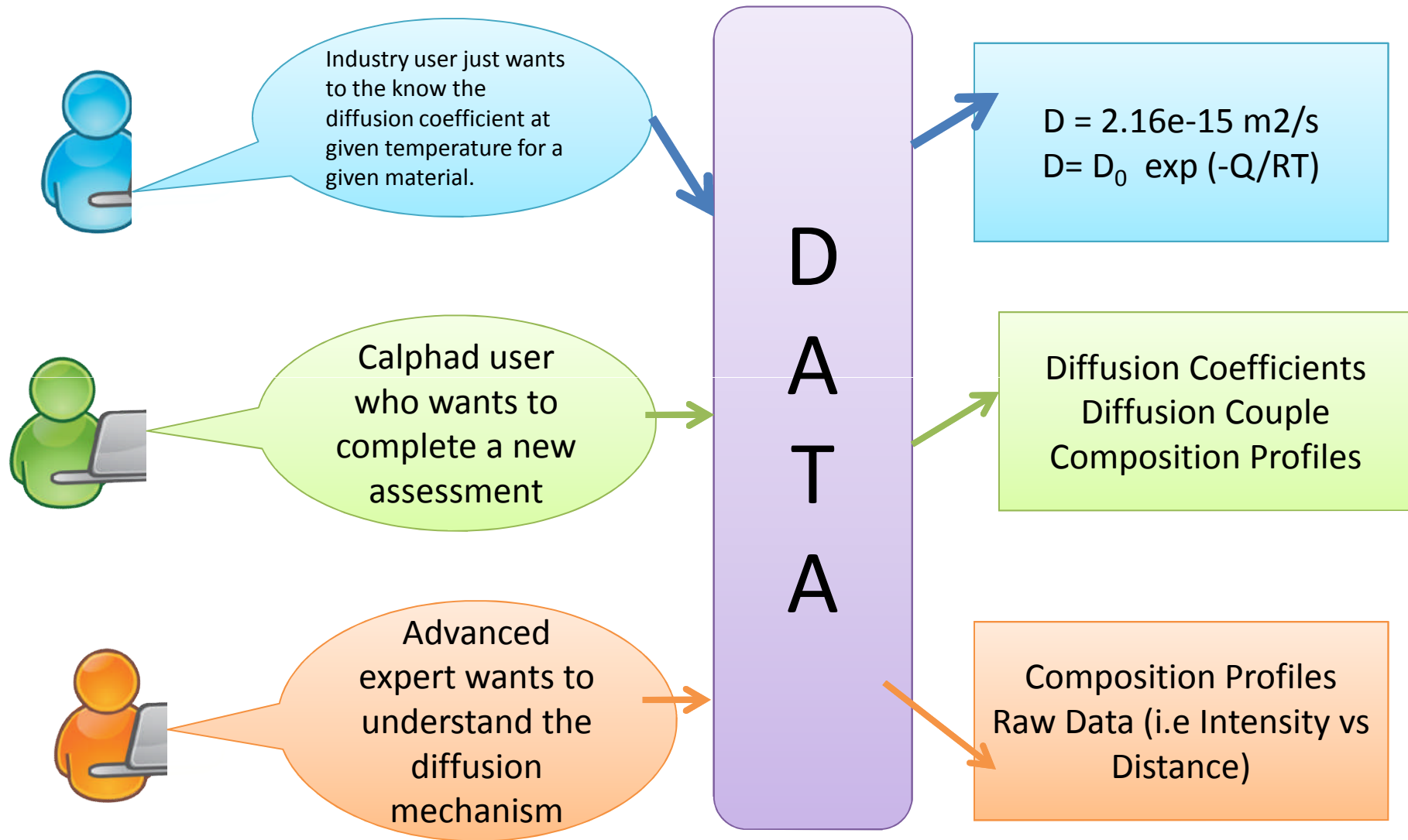
3-D Atom Probe Tomography



Data Dependencies




Different Data Users: Diffusion Data



File Repository/DSpace

OSU http://www.camm.ohio... Inside NIST Add to Wish List Zip Code 20892



NIST
Enable & Enhance **Exchange**
(repositories, disciplines, industries)

NIST File Repositories → NIST File Repositories

NIST File Repositories

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Search within this community and its collections:

The [National Institute of Standards and Technology](#) is establishing essential data protocols and mechanisms to ensure the quality of materials data and models widespread adoption and data sharing.

Collections in this community

- CALPHAD Assessments
- First Principles Phase Stability (FPPS) Files
- Interatomic Potentials

Recent Submissions

Al-Cr-Ni Diffusion Mobilities in Gamma Prime and B2
Campbell, C.E. (2013-02-11)
This work presents the assessment of the diffusion mobilities in both the γ' (Ni₃Al-L12) and B2 (NiAl) phases in the Ni-Al-Cr system utilizing the phenomenological model developed by Helander and Ågren. Available experimental ...

AIN-GaN; GaN-InN; AlN-InN
Burton, Benjamin; van de Walle, Anton; Kattner, Ursula (2013-01-31)
First principles phase diagram calculations were performed for the wurtzite-structure quaternary AIN-GaN, GaN-InN, and AlN-InN.

Al₂O₃ Replication data for cyclic deformation and recovery

Profile: Carelvn Campbell | Logout



NIST
Enable & Enhance **Exchange**
(repositories, disciplines, industries)

NIST
Assess & Improve **Quality**
(data, models, integration, etc.)

NIST File Repositories → NIST Data File Repositories → CALPHAD Assessments

CALPHAD Assessments

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Recent Submissions

Al-Cr-Ni Diffusion Mobilities in Gamma Prime and B2
Campbell, C.E. (2013-02-11)
This work presents the assessment of the diffusion mobilities in both the γ' (Ni₃Al-L12) and B2 (NiAl) phases in the Ni-Al-Cr system utilizing the phenomenological model developed by Helander and Ågren. Available experimental ...

Ni-Al-Cr system Thermodynamic Re-Assessment of the Ternary System Al-Cr-Ni
Dupin, N.; Ansara, I.; Sundman, B. (2013-01-31)
A re-assessment of the ternary system Al-Cr-Ni following Dupin's thesis work using a single Gibbs energy function for the gamma and gamma prime phases is presented taking into account new experimental liquidus temperatures. ...

Ag-Al Functional Description
Du, Zeting; Jing, Zhan-Peng; Li, Changrong; Niu, Chunji (2013-01-31)
The energy expressions for GP zones in the Al-Ag binary system, including the ϵ -state and the η -state ones, are established by combining the essential Gibbs energy for the matrix alloy with the interfacial energy and the ...

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Data Repositories

Different communities have different needs

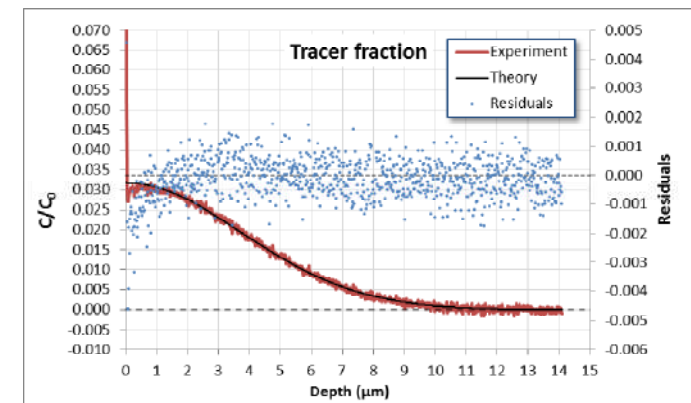
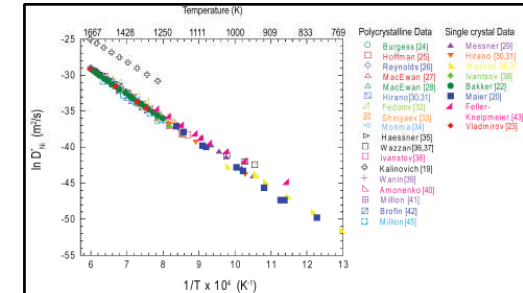
- **Evaluated data**

are needed by most data users as input computational and simulation tools

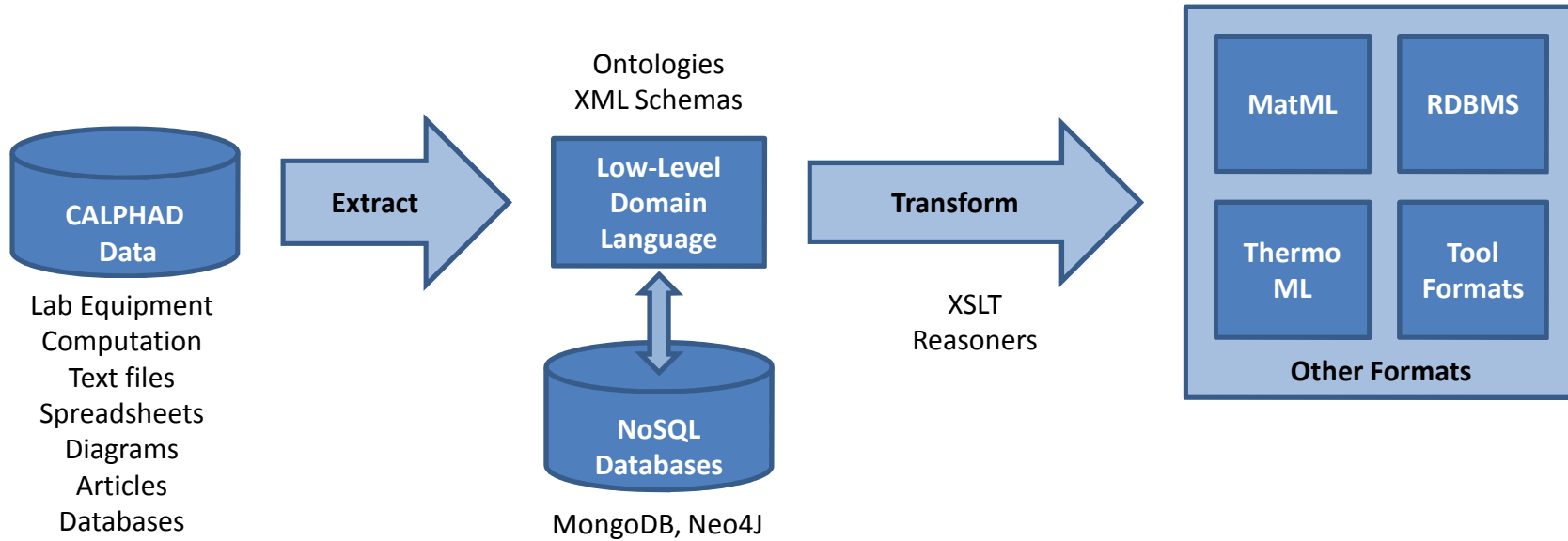
- **Original measured data**

are needed to develop analytical functions

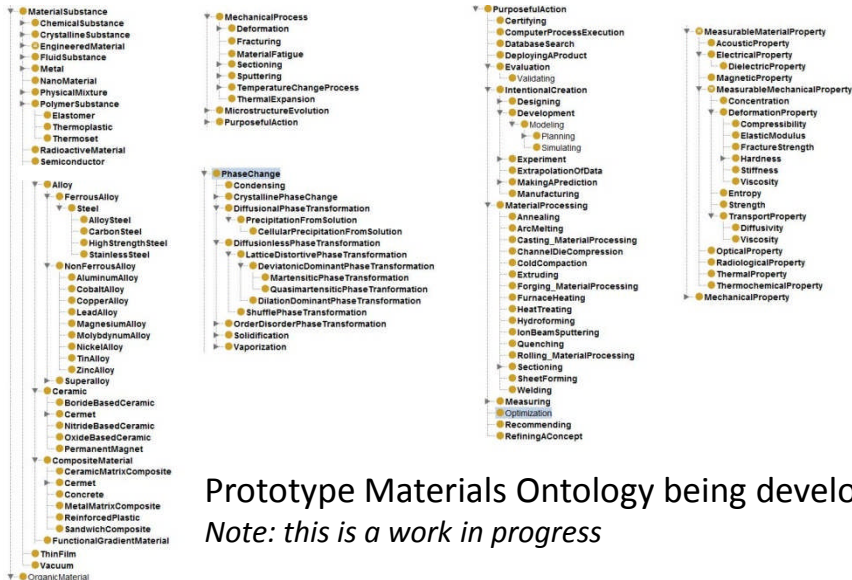
- Ideally one would have a number of sources with original measured data
- These data are in general not available in published papers or at best in graphical form
 - Digitization from graphs creates additional errors!
- Repositories provide the space to accurately store these data for future use



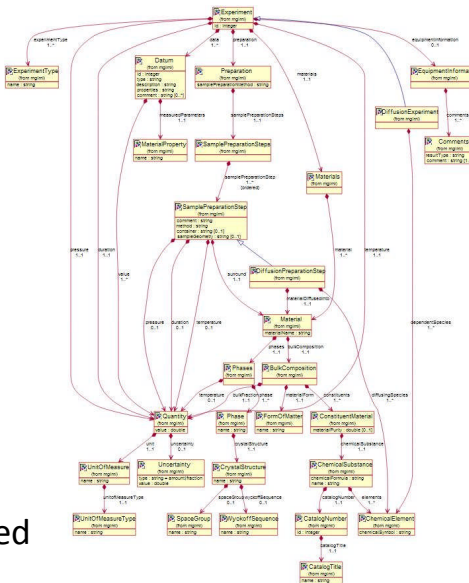
Data Curation



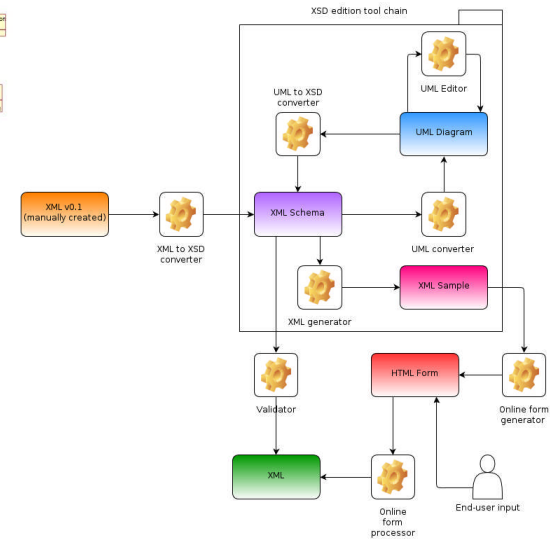
Section of XML Schema



Prototype Materials Ontology being developed
 Note: this is a work in progress



Tool Chain



Data Collection: Tracer Diffusivity Test Schema

Material Genome Initiative
XML Form Editor

Contact us | F.A.Q | Site

Home Register Experiment Data Exploration

Enter Data View XML

Data Entry

In this step, you have to fill in the form. During the process, once you have fill every field, you can view the XML.

Navigation: Home, 1, 2, 3, 4, 5, 6, 7, End

Experiment

- ExperimentType
 - Choose TracerDiffusivity
- Id
- Citation
 - Choose Citation
 - Citation
 - Doi

Navigation: Home, 1, 2, 3, 4, 5, 6, 7, End

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Navigation: Home, 1, 2, 3, 4, 5, 6, 7, End

Experiment

- ExperimentType
 - Choose TracerDiffusivity
- TracerDiffusivity
 - Material
 - MaterialName Mg
 - Phase
 - Name HCP
 - CrystalStructure
 - SpaceGroup
 - SymbolOrNumber
 - WyckoffSequence
 - Sequence
- Composition
 - QuantityUnit mass fraction
- Constituents
 - Element Ac
 - Quantity
 - Purity
 - Error
- MaterialForm
 - Choose SingleCrystalline
 - SingleCrystalline

Navigation: Home, 1, 2, 3, 4, 5, 6, 7, End

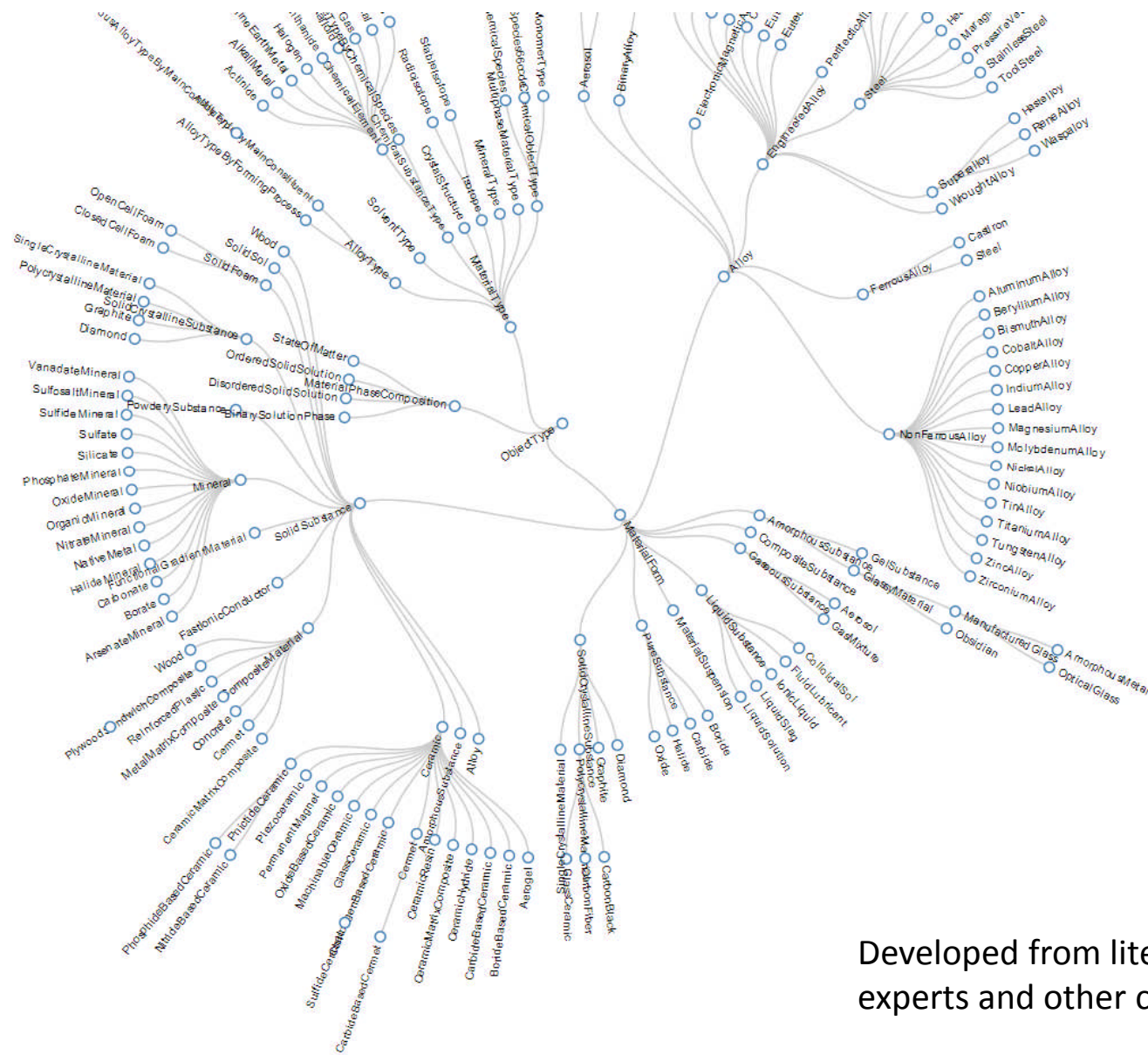
Navigation: Home, 1, 2, 3, 4, 5, 6, 7, End

Experiment

- ExperimentType
 - Choose TracerDiffusivity
- TracerDiffusivity
 - DiffusingSpecies
 - Element Ac
 - MaterialPurity
- ExperimentalConditions
 - MeasurementConditions
 - Time
 - Duration
 - Unit years
 - Uncertainty
 - Type amount
 - Value
 - Temperature
 - Temperature
 - Unit Kelvin
 - Uncertainty
 - Type amount
 - Value
 - Environment
 - Environment

Navigation: Home, 1, 2, 3, 4, 5, 6, 7, End

Prototype MGI Ontology



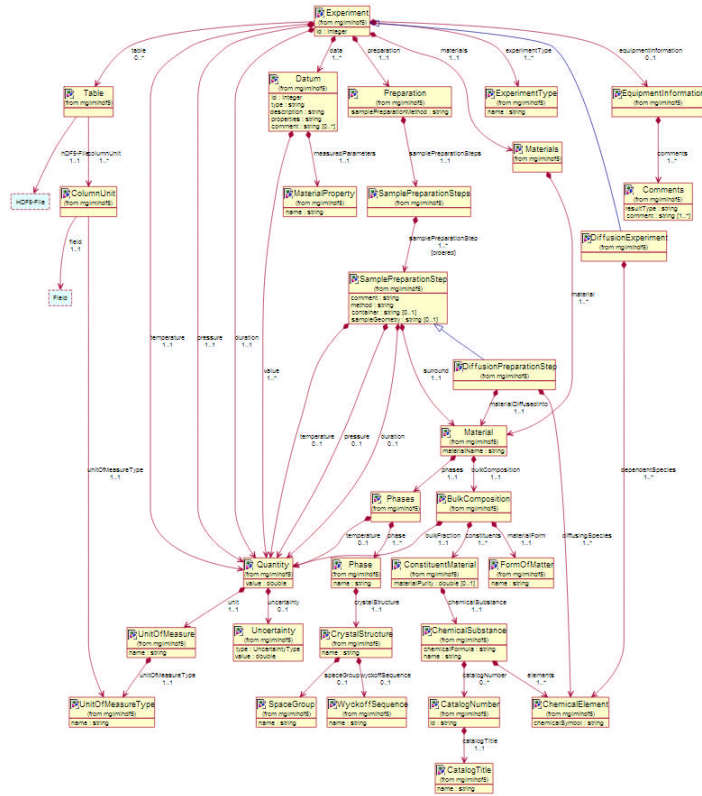
Broad concepts covered in materials data files (data have many types)

- Objects, Materials, and Events
- Physical Properties
- Documents
- Data Objects & Types
- People & Organizations
- Software
- Relations among these

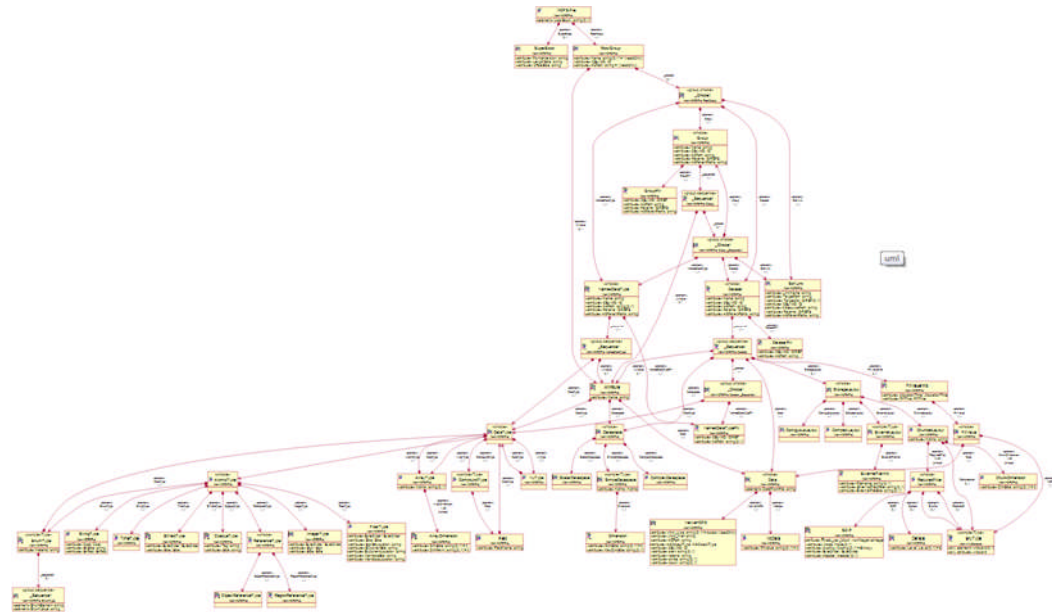
Developed from literature supplied by domain experts and other community resources

Encoding CALPHAD Data

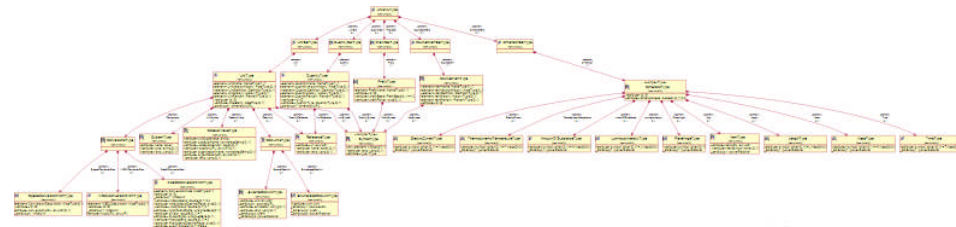
Core CALPHAD



Tabular Data (HDF5)



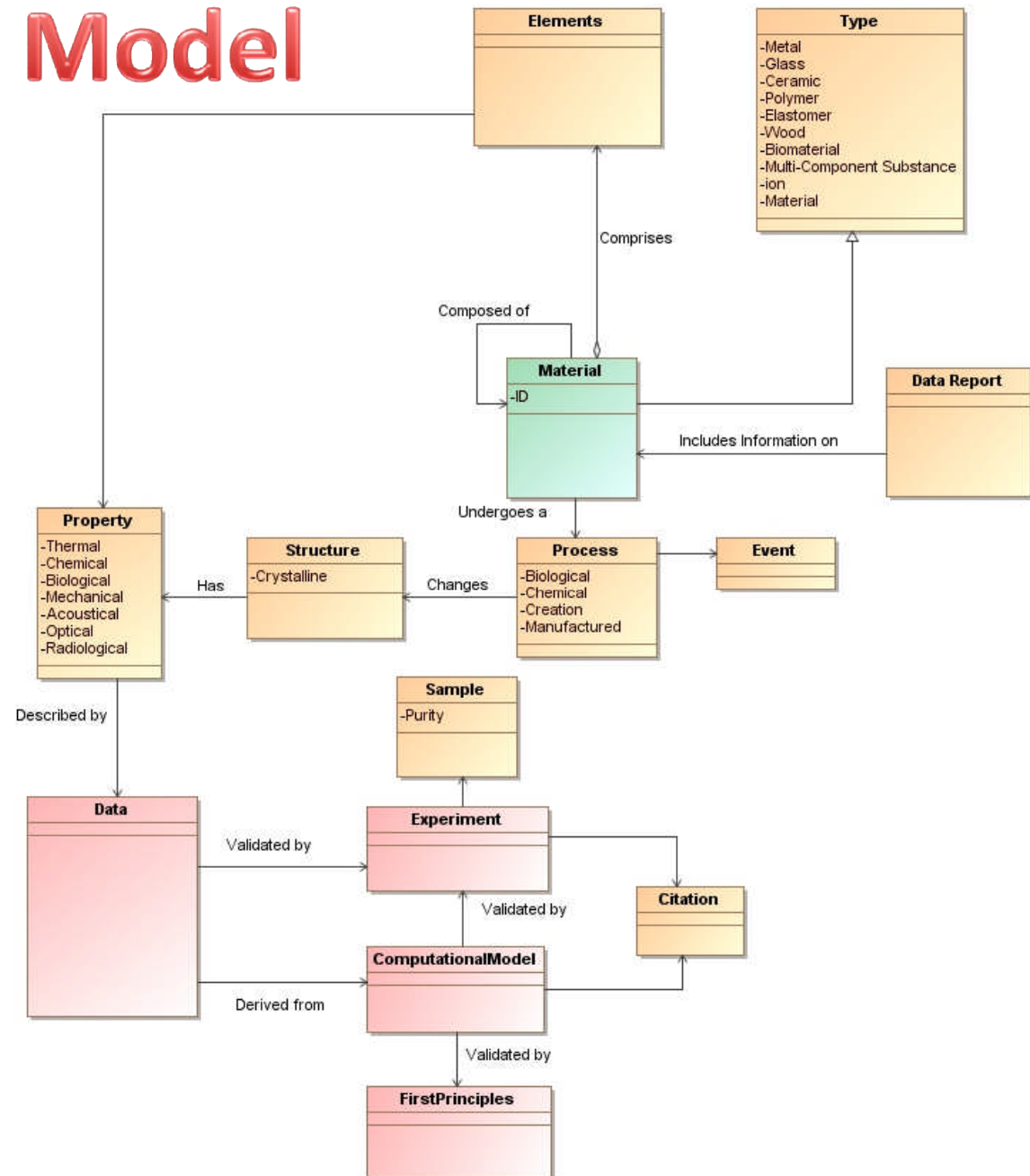
Measurement Units (Units ML)



UML Domain Model

Sources

- Prototype MGI Ontology
- ThermoML
- MatML
- MatSeek
- UnitsML
- ChemML



Questions for the Panel

- Prototype ontology
 - How do we evaluate it?
 - How do we best proceed with its development?
 - What tools are available to support community-based efforts?
 - What is the best way for us to encode our ontology?
- Graph databases
 - Any advice for using property graphs to represent ontologies?
- Software development and ontology
 - How do we best integrate ontology with UML?
 - What is the relationship between ontology and UML domain models?
- Community Experience
 - Are there examples of similar ontology-based systems for us to compare?