

Data Informatics and Tools

C. E. Campbell, U.R. Kattner, Material Measurement Laboratory,
NIST

A. Dima, Information Technology Laboratory, NIST

Laura Bartolo, Kent State University

NIST Diffusion Workshop

May 9, 2013

Our Collaborators

NIST Information Technology Laboratory

Information Systems Group

Y.-S. Li-Baboud, P. Dessauw, P. Savonitto, D. Foxvog

NIST Material Measurement Laboratory

Technical Program Director for Materials Genomics

J.A. Warren

Thermodynamics and Kinetics Group

B.P. Burton, R.H. Taylor, C.A. Becker, F. Tavazza

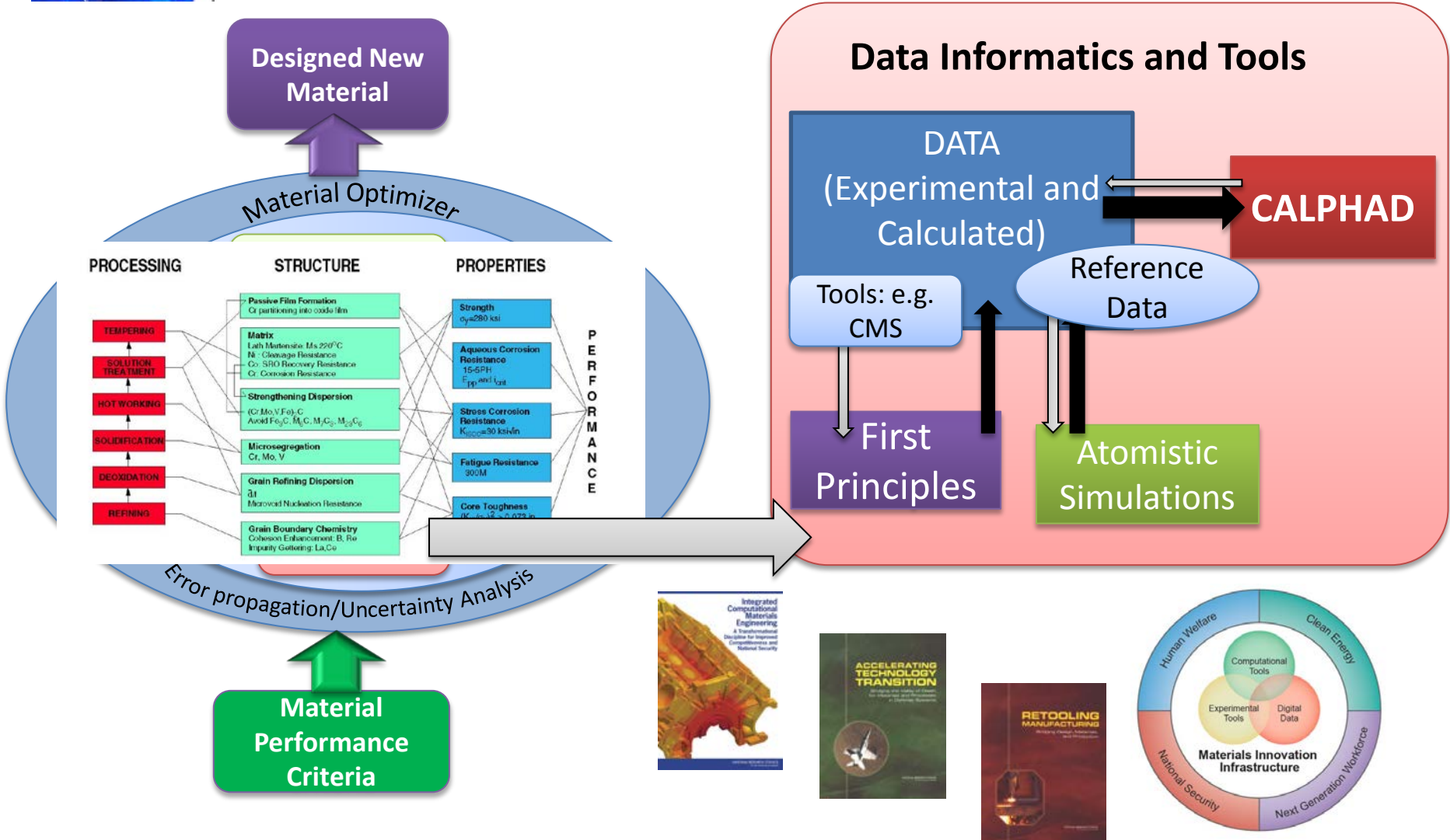
Cell Systems Science Group

T.N. Bhat, J.T. Elliott



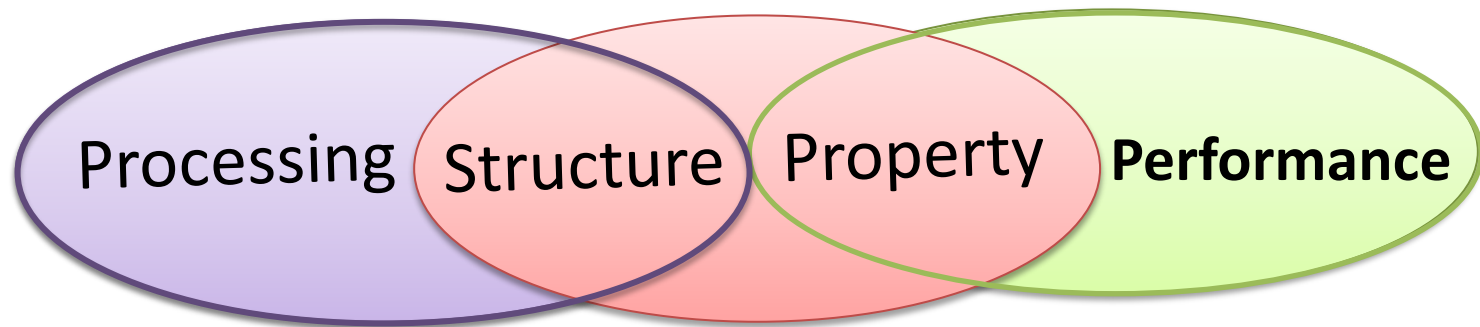
Materials Genome Initiative: The Need for Data and Informatics

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

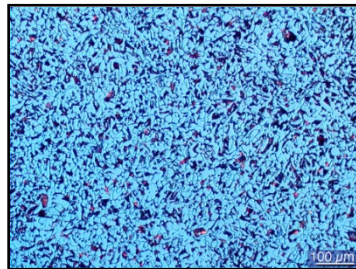
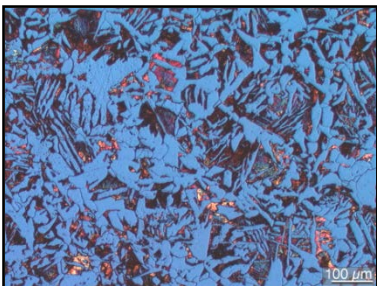


Materials Are Complicated Hierarchical Systems

- 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



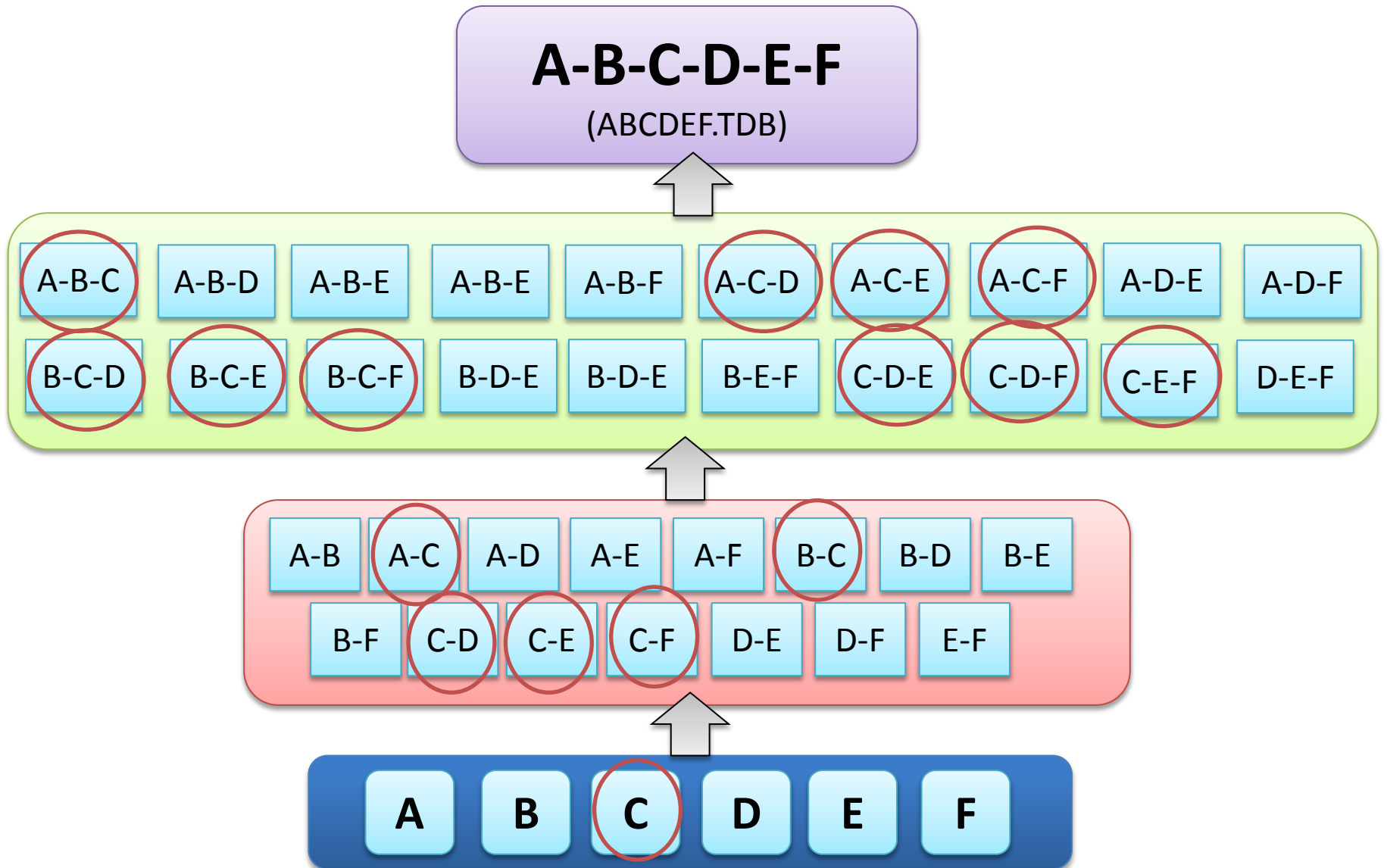
Material A at Temp. 2

Key to material design:

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

 **CALPHAD**

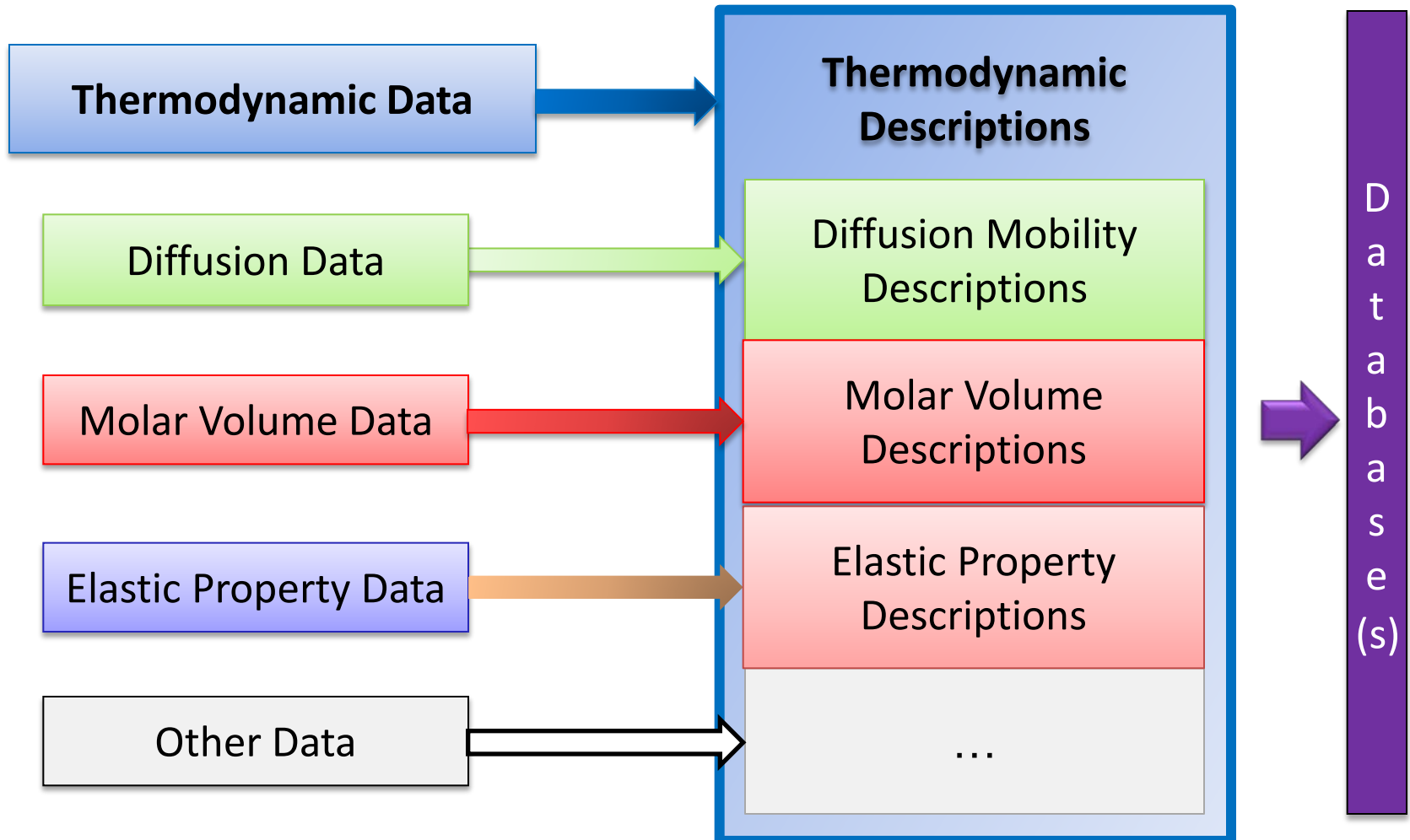
Data Dependencies



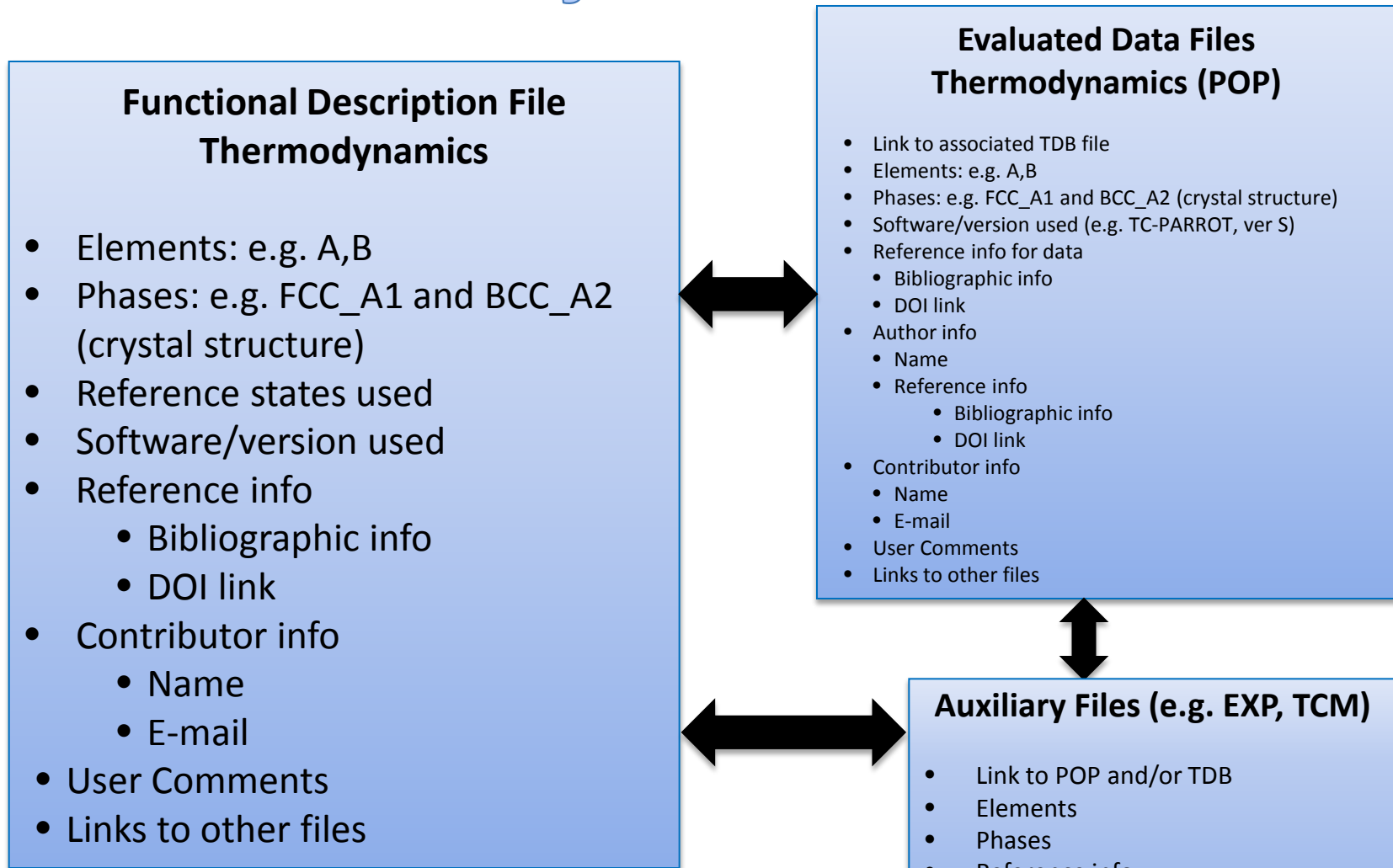
Data Flow of CALPHAD “Database” Files

Evaluated Data Files
(e.g. POP, DOP)

Functional Descriptions
(e.g. TDB)



Examples of Files for a CALPHAD Thermodynamic Assessment



Note: Thermo-Calc based file extensions used, but information on file types should also be included

EXAMPLES OF FILES FOR A CALPHAD: DIFFUSION MOBILITY ASSESSMENT

Database files

Thermodynamic Description

Link to
TDB file or
reference

Diffusion Mobility Description

- Elements: e.g. A,B
- Phases: e.g. FCC_A1 and BCC_A2 (crystal structure)
- Software/version used
- Reference info
 - Bibliographic info
 - DOI link
- Contributor info
 - Name
 - E-mail
- User Comments
- Links to other files

Evaluated Data Files (e.g.DOP)

- Link to associated TDB file
- Elements: e.g. A,B
- Phases: e.g. FCC_A1 and BCC_A2 (crystal structure)
- Software/version used (e.g. TC-PARROT, ver S)
- Reference info for data
 - Bibliographic info, DOI link
- Author info
 - Name
 - Reference info
 - Bibliographic info, DOI link
- Author info
 - Name, e-mail
- User Comments
- Links to other files

MACRO/Script Files (e.g. to run simulations , DCM)

- Elements
- Phases
- Reference
- Author
- Links to other files (grid data, start values)
- User comments

Auxiliary Data Files (e.g. *.EXP)

- Link to POP and/or TDB
- Elements
- Phases
- Reference info
- Author
- Links to other files
- User comments

Note: Thermo-Calc based file extensions used, but information on file types should also be included

Selecting a Repository System

- **Must provide**

- the ability to link files
- tags for properties, phases and models,
- customize metadata
- search capability
- customization with own tools
- the ability to link with other repository systems
- **persistent identifiers for data**
- **License for data use**



- Must be flexible enough to adapt to future needs
- Must be easy to use and install

- **Systems explored**



} Free Software

Populating the Repository

Tags are needed to facilitate searches and provide information about the system and the file contents!



The effort required to populate repository must be minimal to be attractive for contributions from the community!



Essential Tags:

- Elements
- Reference
- Property (thermodynamics, diffusion, ...)
- Phases

Suggested Common Tags for CALPHAD; First Principles and Atomistics

- **Methods**

- First-Principles
- Atomistics
- CALPHAD
- Other

- **Property Type**

- Thermodynamic
- Kinetic
- Molar Volume
- Mechanical
- Electrical
- Optical
- Magnetic
- Interface/Surface
- Other*

- **Systems**

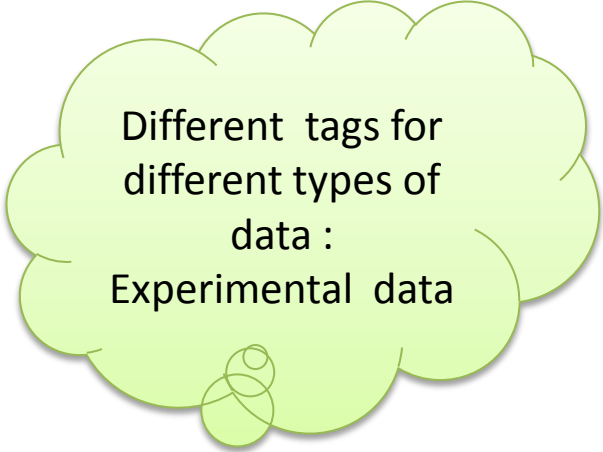
- **A-G**
 - Al Binaries
 - Al Ternaries
 - Al High Order Systems
- **H-L**
-

- **State**

- Gas
- Liquid
- Other
- Solid
 - Bulk
 - Nano
 - Phases

- **Software**

- **First Principles**
 - VASP
 - DMOL
 - ABINIT
 - SIESTA
 - WIEN2k
 - Materials Studio
 - *other*



Different tags for different types of data :
Experimental data

- **CALPHAD**

- Thermo-Calc
- Pandat
- FactSage
- OC
- MTData
- *other*

- **ATOMISTICS**

- LAMMPS
- IMD
- *other*

Suggested Common Tags for Experiments

- **Alloy Class**

-

- **Mg Alloys**

- Cast Alloys

- Mg-Al
- Mg-Al-Mn
- Mg-Al-Zn
- Mg-Al-RE (RE-Rare Earth)

- Wrought Alloys

- Mg-Al
- Mg-Li
- Mg-Zn

- **Systems**

- **A-G**

- Al Binaries
- Al Ternaries
- Al High Order Systems

- **H-L**

-

- **State**

- Gas
- Liquid
- Other
- Solid (Bulk; Nano; Phase)

- **Property Type**

- **Thermodynamic**

- Enthalpy
- Activity/chemical potential
- Heat Capacity
- Phase Equilibria
 - » Phase boundaries
 - » Transition temperature
 - » Single phase defect

- **Kinetic**

- Diffusivities
 - Tracer
 - Intrinsic
 - Interdiffusion
- Nucleation

- **Molar Volume**

- Lattice parameters
- Thermal Expansion

- **Mechanical**

- **Electrical**

- **Thermal Conductivity**

- **Optical**

- **Magnetic**

- Interface/Surface
- Corrosion
 - Potential-pH (Pourbaix) diagrams
 - Polarization measurements
 - Electrochemical measurements
 - Corrosion rates
- *Other*

Suggested Common Tags for Experiments

• Experimental Methods

- Image Analysis
 - Optical Metallography
 - SEM
 - TEM
 - Atom Probe
- X-Ray Diffraction
- Dilatometry
- Calorimetry
 - Differential Scanning Calorimetry
 - Solution
 - Drop
 - Other
- Differential Thermal Analysis
- Electromotive Force
- Vapor pressure
 - Knudsen
 - Other
- Composition Analysis
 - Electron Probe Microanalysis
 - SIMS

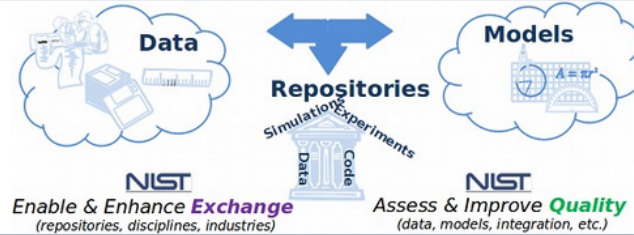
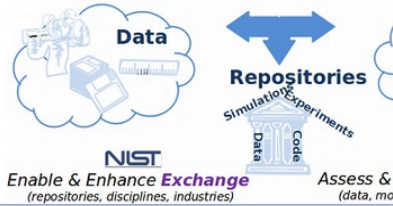
• Processing

- Casting
 - Centifugal
 - Die
 - Investment
 - Sand/mold
- Deformation
 - Drawing
 - Extrusion
 - Forging
 - Rolling
 - Sheet
- Machining
 - Abrasive
 - Electrical/chemical
 - Machining (i.e. Drilling , Milling)
 - Sheet/film (punching, perforating,)
- Thermal
 - Electron beam Machining
 - Laser cutting
 - Plasma arc cutting

- Molding
 - Blow
 - Calendering
 - Compression
 - Injection
- Powder Processing
 - Cold
 - Hot
- Thermal Processing
 - Homogenization
 - Aging

File Repository/DSpace

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



Profile: Carelyn Campbell | Logout

NIST File Repositories → NIST File Repositories

NIST File Repositories → NIST Data File Repositories → CALPHAD Assessments

NIST File Repositories

Browse by

- [By Issue Date](#)
- [Authors](#)
- [Titles](#)
- [Subjects](#)

Search within this community and its collections:

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

[AlN-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 quasis AlN-GaN, GaN-InN, and AlN-InN.

[Au Replication data tensile deformation gold nanowires](#)

CALPHAD Assessments

Browse by

- [By Issue Date](#)
- [Authors](#)
- [Titles](#)
- [Subjects](#)

Search within this collection:

[Submit a new item to this collection](#)

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 ...

Search DSpace

- Search DSpace
- This Collection

[Advanced Search](#)

Browse

All of DSpace

[Communities & Collections](#)

[By Issue Date](#)

[Authors](#)

[Titles](#)

[Subjects](#)

This Collection

[By Issue Date](#)

[Authors](#)

[Titles](#)

[Subjects](#)

My Account

[Logout](#)

[Profile](#)

[Submissions](#)

Context

[Edit Collection](#)

[Item Mapper](#)

[Export Collection](#)

[Export Metadata](#)

Statistics

[View Usage Statistics](#)

[View Search Statistics](#)

[View Workflow Statistics](#)

Discover

Sample Entry

Data Citation

NIST File Repositories (repositories, disciplines, industries) (data, models, innovation, etc.)
NIST File Repositories → NIST Data File Repositories → CALPHAD Assessments → View Item

CALPHAD Assessments

Browse by

- By Issue Date
- Authors
- Titles
- Subjects

Search within this collection:

[Submit a new item to this collection](#)

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 phases in the Ni-Al-Cr system utilizing the phenomenological model developed by Helander and Agren. Available experimental tracer diffusivity, interdiffusion coefficients and activation energies were evaluated and then used to optimize the composition- and temperature-dependent diffusion mobilities. For both the B₂ and γ' phases, the assessed diffusion mobility descriptions reproduce the Arrhenius temperature dependence for the Ni, Al and Cr tracer diffusivities and interdiffusion coefficients. The assessment reproduces the strong composition dependence of the diffusivities in the B₂ phase observed experimentally. The measured composition dependences of the diffusivities in the γ' phase are also replicated by the present mobility descriptions. The assessed mobility descriptions are validated by comparing calculated and measured composition profiles for a variety of Ni-Al and Ni-Al-Cr diffusion couples, including B₂/B₂, γ' (fcc)/ γ' and γ' /B₂ couples.

[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 energy function for the gamma and gamma prime phases is presented taking into account experimental liquidus temperatures. ...

[Ag-AI Functional Description](#)

Du, Zefeng; 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 δ -ones, are established by combining the essential Gibbs energy for the matrix alloy with the interfacial energy and the ...

Data Citation:
Al-Cr-Ni Diffusion Mobilities in Gamma Prime and B2
Campbell, C.E.
<http://hdl.handle.net/11119/51>

Affiliation: Metallurgy Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8555, USA
Contact Email: carelyn.campbell@nist.gov

Publication Citation:

Campbell, C.E. "Assessment of the diffusion mobilities in the gamma prime and B2 phases in the Ni-Al-Cr system," *Acta Mater.* 2008,56:4277.
<http://dx.doi.org/10.1016/j.actamat.2008.04.051>

Related Work:

Dupin, N.; Ansara, I.; Sundman, B. "Thermodynamic Re-Assessment of the Ternary System Al-Cr-Ni" CALPHAD 2001;25:279. Publication: [http://dx.doi.org/10.1016/S0364-5916\(01\)00049-9](http://dx.doi.org/10.1016/S0364-5916(01)00049-9) Data: <http://hdl.handle.net/11119/51>

Similar Work:

Zhang, J.; Du, Y.; Chen, Q.; Steinbach, J. "Atomic mobilities and diffusivities in the fcc, L1₂ and B₂ phases of the Ni-Al system," *International Journal of Materials Research*, 2010;146:1. <http://dx.doi.org/10.3139/I146.110428>

Abstract:

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 Agren. Available experimental tracer diffusivity, interdiffusion coefficients and activation energies were evaluated and then used to optimize the composition- and temperature-dependent diffusion mobilities. For both the B₂ and γ' phases, the assessed diffusion mobility descriptions reproduce the Arrhenius temperature dependence for the Ni, Al and Cr tracer diffusivities and interdiffusion coefficients. The assessment reproduces the strong composition dependence of the diffusivities in the B₂ phase observed experimentally. The measured composition dependences of the diffusivities in the γ' phase are also replicated by the present mobility descriptions. The assessed mobility descriptions are validated by comparing calculated and measured composition profiles for a variety of Ni-Al and Ni-Al-Cr diffusion couples, including B₂/B₂, γ' (fcc)/ γ' and γ' /B₂ couples.

Files in this item

- | | | |
|--|--|---------------------------|
| | Name: exp-b2.zip
Size: 9.374Kb
Format: application/zip
Description: Experimental data for NiAl B2 phase | View/Open |
| | Name: exp-ni3al.zip
Size: 9.619Kb
Format: application/zip
Description: Experimental diffusion data files for Ni3Al | View/Open |
| | Name: alcrni-mob-NIST-0 ...
Size: 57.23Kb
Format: application/zip
Description: Diffusion mobility description for Ni-Al-Cr using N. Dupin thermodynamics (CALPHAD 2001) | View/Open |
| | Name: Re-assessment-112 ...
Size: 237.1Kb
Format: PDF
Description: Expansion of revision to publication on diffusion mobility description. | View/Open |

The following license files are associated with this item:

- [Creative Commons](#)

Digital Identifier

Related Work

Similar Work

Data files

Offer licenses with attribution 3.0



Current Advance Search Options

NIST File Repositories → Filter by: Subject

[A](#)[B](#)[C](#)[D](#)[E](#)[F](#)[G](#)[H](#)[I](#)[J](#)[K](#)[L](#)[M](#)[N](#)[O](#)[P](#)[Q](#)[R](#)[S](#)[T](#)[U](#)[V](#)[W](#)[X](#)[Y](#)[Z](#)

Starts with

Filter by: Subject

Now showing items 1-10

[Next Page](#)

[Au \(Gold\) \(1\)](#)

[Chemical Systems \(4\)](#)

[Chemical Systems::AG \(Silver\) \(1\)](#)

[Chemical Systems::AG \(Silver\)::Ag Binaries \(1\)](#)

[Chemical Systems::Al \(Aluminum\) \(4\)](#)

[Chemical Systems::Al \(Aluminum\)::Al Binaries \(2\)](#)

[Chemical Systems::Al \(Aluminum\)::Al Higher Ordered \(2\)](#)

[Chemical Systems::Cr \(Chromium\) \(2\)](#)

[Chemical Systems::Cr \(Chromium\)::Cr Higher Ordered \(2\)](#)

[Chemical Systems::Ga \(Gallium\) \(1\)](#)

Now showing items 1-10

[Next Page](#)

DSpace software copyright © 2002-2012

[Contact Us](#) | [Send Feedback](#)

NIST File Repositories → Filter by: Subject

[A](#)[B](#)[C](#)[D](#)[E](#)[F](#)[G](#)[H](#)[I](#)[J](#)[K](#)[L](#)[M](#)[N](#)[O](#)[P](#)[Q](#)[R](#)[S](#)[T](#)[U](#)[V](#)[W](#)[X](#)[Y](#)[Z](#)

Starts with

Filter by: Subject

Now showing items 21-25

[Phases::Liquid \(1\)](#)

[Platforms \(1\)](#)

[Platforms::Thermocalc \(1\)](#)

[Property Classes \(2\)](#)

[Property Classes::Thermodynamics \(2\)](#)

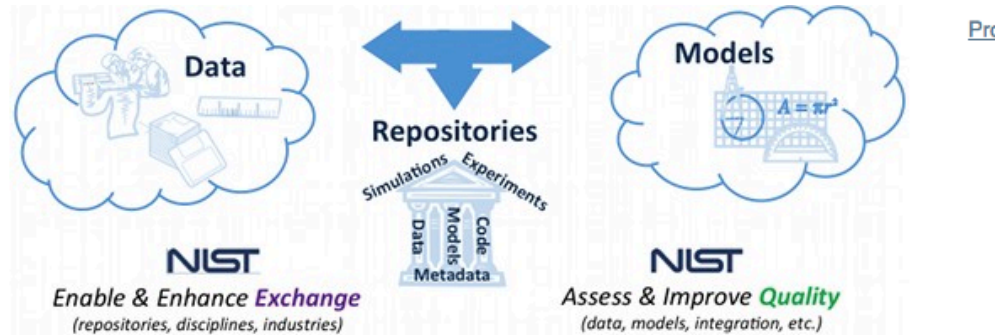
Now showing items 21-25

DSpace software copyright © 2002-2012

[Contact Us](#) | [Send Feedback](#)

Tag/Search Terms will eventually will be tie to ontology

Upload & Embargo Unpublished Data



Data submission



Access Settings

Private Item:

If selected, the item won't be searchable



Embargo Access until Specific Date:

Accepted format: yyyy, yyyy-mm, yyyy-mm-dd

Reason:

Search NIST

Search NIST

This Collection

[Advanced Search](#)

Browse

All of NIST Re

[Communiti](#)

[Subjects](#)

[Titles](#)

[Authors](#)

This Collection

[Subjects](#)

[Titles](#)

[Authors](#)

My Account

[My Exports](#)

[Logout](#)

[Profile](#)

[Submissions](#)

Creative Commons 3.0 with 4 versions

<http://creativecommons.org/licenses/>

Attribution:

You must attribute the work in the manner specified by the author or licensor. (Not to be used for endorsements)

4 versions of 3.0 License allows one to choose:

- To share, adapt, & make commercial use of work.
- To share, adapt & no commercial use of work
- To share, adapt, make commercial use of work & share alike.
- To share, adapt, no commercial use of work & share alike.

Share — Copy, distribute, and transmit work

Share Alike — re-distribution & re-use of licensed work under the same, similar or a compatible license.

Waiver — Any of the above conditions can be [waived](#) if you get permission from the copyright holder.

Public Domain — Where the work or any of its elements is in the [public domain](#) under applicable law, that status is in no way affected by the license.

Other Rights — In no way are any of the following rights affected by the license:

Your fair dealing or [fair use](#) rights, or other applicable copyright exceptions and limitations;

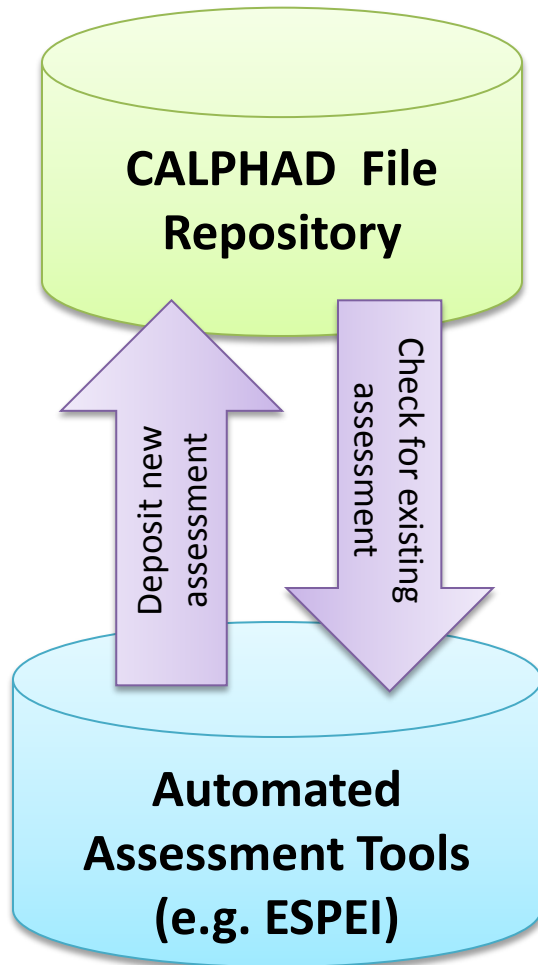
The author's [moral](#) rights;

Rights other persons may have either in the work itself or in how the work is used, such as [publicity](#) or privacy rights.

Notice — For any reuse or distribution, you must make clear to others the license terms of this work. The best way to do this is with a link to this web page.

Improving the CALPHAD Assessment Process

**What if the evaluated data file (e.g. POP) is missing?
Are there new experimental or computational data?**



Requires data search

Examples of CALPHAD Data Types

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

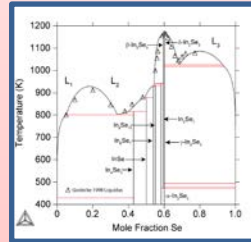
Functional descriptions for phase quantity (e.g. TDB)

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

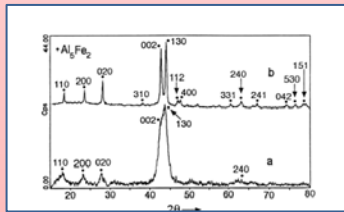
1-D (Points)

Melting Temperatures

Critical Temperatures
(Phase Changes)



Lattice Parameters



Heat of Formations

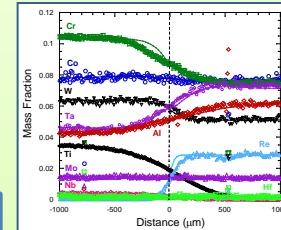
Phase fractions and
compositions

Tracer
Diffusivities

Activation energies

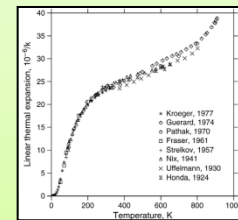
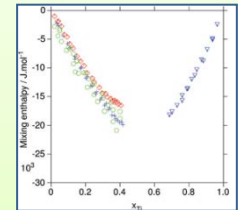
2-D (Lines)

Composition
Profiles



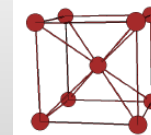
Heat Capacities

Enthalpies of mixing

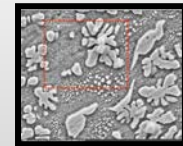


3-D

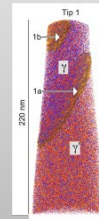
Crystal structures



Micrographs/Morphologies



3-D Atom probe Tomography



Example Information Needed to Describe General Data Entry

Data

- Elements present
- Type of value (e.g. enthalpy, heat of formation, phase boundary, diffusivity, lattice parameter, bulk modulus)
 - Experimental or computational method
 - Type of measurement (direct or indirect)
- Number of phases present
- Datum value and error
 - Type (single value or series)
 - Units
 - Actual value(s) and error(s)
- For each phase present
 - Phase name
 - Composition and fraction and errors
 - Crystal structure (this input will follow the format prescribed by the CCN) or amorphous
 - Lattice parameter
- Temperature and error
- Pressure and error
- Type of Material
 - Bulk composition
 - Material purity
 - Sample preparation
 - Microstructure information
 - Single crystal
 - Polycrystalline (grain size, dislocation density)
 - Non-crystalline

**Need extensible formats
that can evolve with
changing data needs!**

Metadata

- Data manipulation details (if any, e.g. reference state corrections, analysis method to determine interdiffusion coefficient)
- Reporting format (raw data, digitized data, other)
- Reference (DOI or text ; one must be present)
- Additional information

Phase-Based Property Database

➤ Material Property Database Exist

GRANTA
MATERIAL INTELLIGENCE

**MATERIALS
PROJECT**

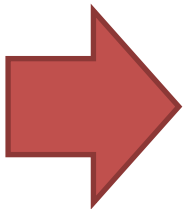
 **MatWeb**

ASN
INTERNATIONAL
The Materials
Information Society
**Everything
Material.**

 **MatNavi**

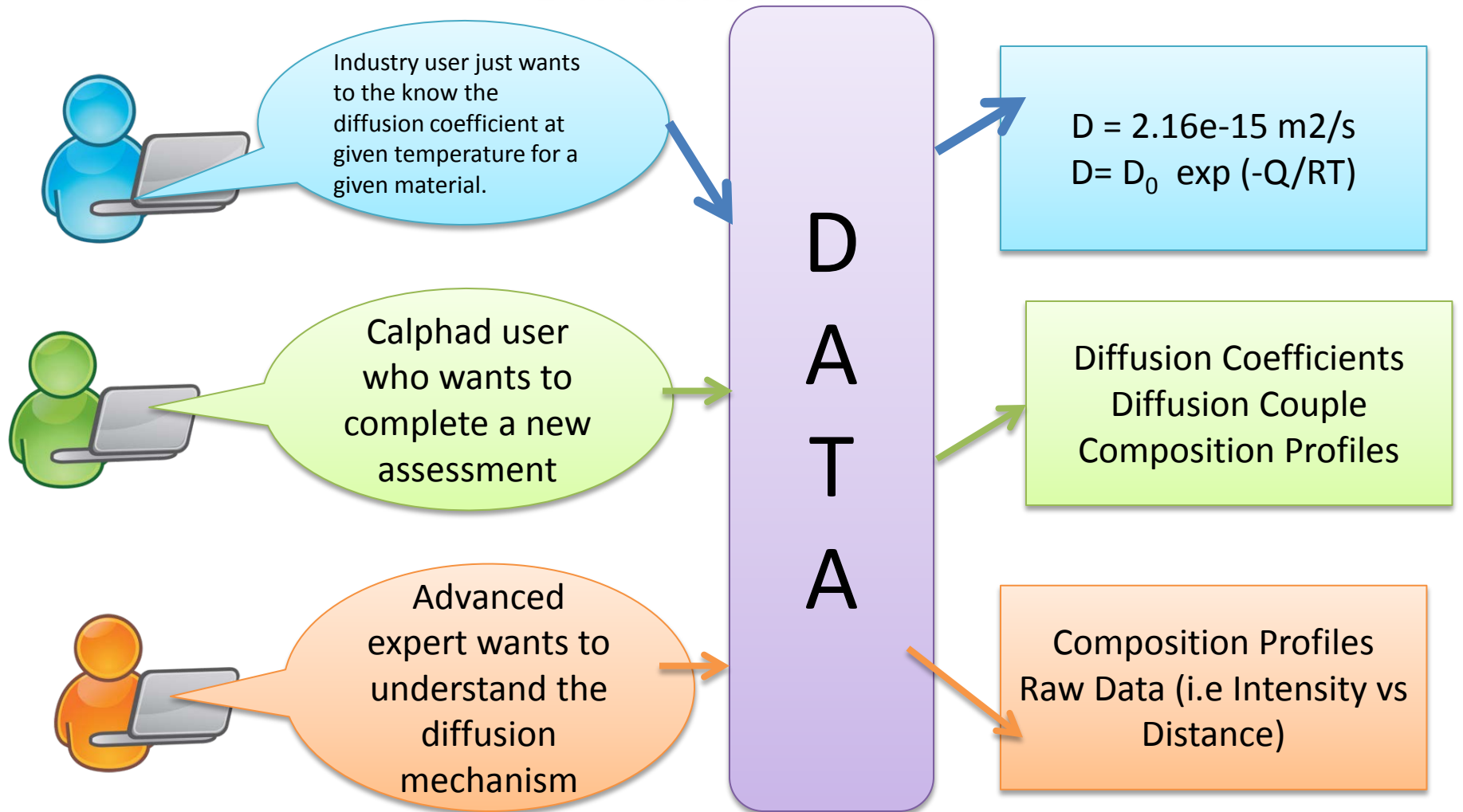
AFLOWLIB.ORG

Generally, focused on engineering/design specs or first-principle calculations results.



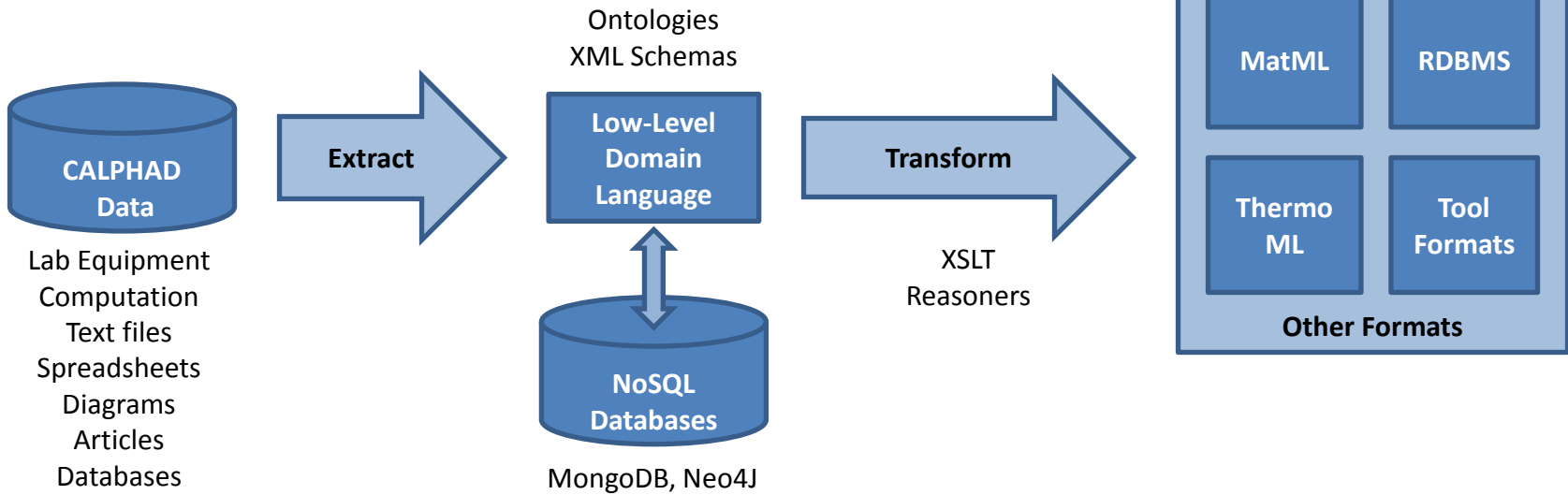
- **Focus on phase-based properties that are needed to describe the composition, temperature, and pressure functions of a phase.**
- **Unary, binary and ternary data are primary focus.**
- **Multicomponent data are needed for validation**

Example of Different Types of Data Users: Diffusion Data

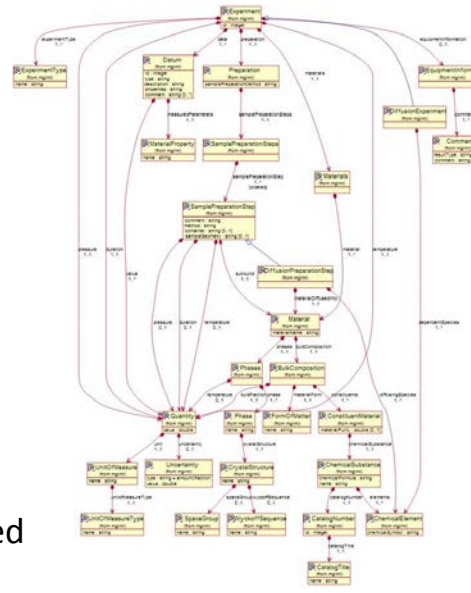


Data are diverse **Data are semi-structured** **Need complete data sets**

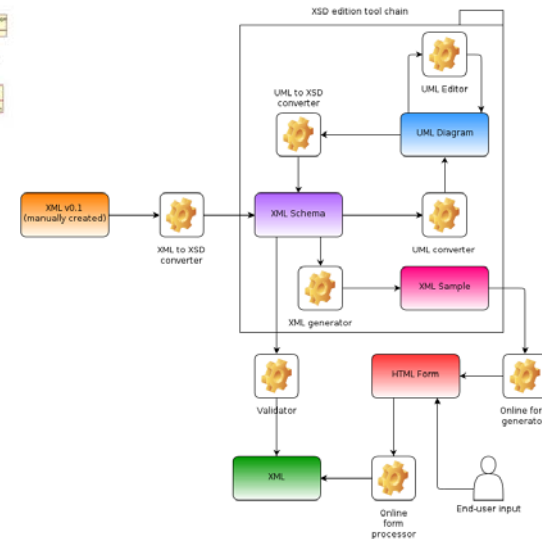
Informatix Approach



Section of XML Schema



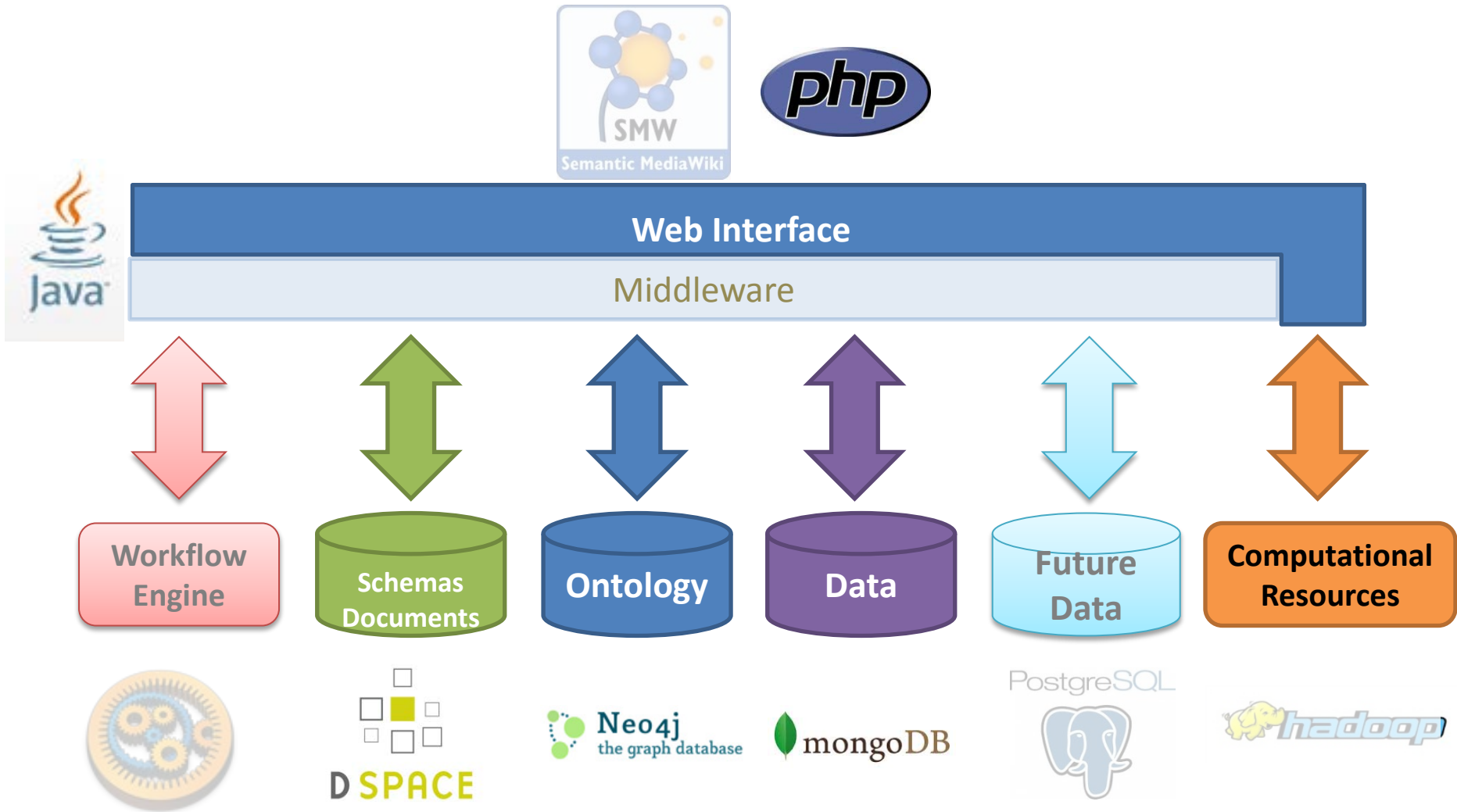
Tool Chain



- Material Substance
 - Chemical Substance
 - Crystalline Substance
 - Engineered Material
 - Fluid Substance
 - Metal
 - NanoMaterial
 - Physical Mixture
 - Polymer Substance
 - Elastomer
 - Thermoplastic
 - Thermoset
 - Radioactive Material
 - Semiconductor
- Alloy
 - Ferrous Alloy
 - Steel
 - Alloy Steel
 - Carbon Steel
 - High Strength Steel
 - Stainless Steel
 - NonFerrous Alloy
 - Aluminum Alloy
 - Cobalt Alloy
 - Copper Alloy
 - Lead Alloy
 - Magnesium Alloy
 - Molybdenum Alloy
 - Nickel Alloy
 - Titanium Alloy
 - Zinc Alloy
 - Superalloy
 - Ceramic
 - Boride Based Ceramic
 - Cermet
 - Nitride Based Ceramic
 - Oxide Based Ceramic
 - Permanent Magnet
 - Composite Material
 - Ceramic Matrix Composite
 - Cermet
 - Concrete
 - Metal Matrix Composite
 - Reinforced Plastic
 - Sandwich Composite
 - Functional Gradient Material
 - Thin Film
 - Vacuum
 - Organic Material
- Mechanical Process
 - Deformation
 - Fracturing
 - Material Fatigue
 - Sectioning
 - Sputtering
 - Temperature Change Process
 - Thermal Expansion
 - Microstructure Evolution
 - Purposeful Action
- Phase Change
 - Condensing
 - Crystalline Phase Change
 - Diffusional Phase Transformation
 - Precipitation From Solution
 - Cellular Precipitation From Solution
 - Diffusionless Phase Transformation
 - Lattice Distortive Phase Transformation
 - Deviatonic Dominant Phase Transformation
 - Martensitic Phase Transformation
 - Quasi Martensitic Phase Transformation
 - Dilution Dominant Phase Transformation
 - Order Disorder Phase Transformation
 - Vaporization
- Purposeful Action
 - Certifying
 - Computer Process Execution
 - Database Search
 - Deploying Product
 - Evaluation
 - Validating
 - Intentional Creation
 - Designing
 - Modeling
 - Planning
 - Simulating
 - Development
 - Experiment
 - Extrapolation Of Data
 - Making Prediction
 - Manufacturing
 - Material Processing
 - Annealing
 - Arc Melting
 - Casting_Material Processing
 - Channel Die Compression
 - Cold Compaction
 - Extruding
 - Forging_Material Processing
 - Furnace Heating
 - Heat Treating
 - Hydroforming
 - Ion Beam Sputtering
 - Quenching
 - Rolling_Material Processing
 - Sectioning
 - Sheet Forming
 - Welding
 - Measuring
 - Optimization
 - Recommending
 - Retaining Concept
- Measurable Material Property
 - Acoustic Property
 - Electrical Property
 - Dielectric Property
 - Magnetic Property
 - Measurable Mechanical Property
 - Compressibility
 - Elastic Modulus
 - Fracture Strength
 - Hardness
 - Stiffness
 - Viscosity
 - Entropy
 - Strength
 - Transport Property
 - Optical Property
 - Radiological Property
 - Thermal Property
 - Thermochemical Property
 - Mechanical Property

Materials Ontology currently being developed
 Note this is a work in progress

Architectural Strategy



Benefits from an Ontological Approach

- Semantic Unification
 - The unification of lexically different representations that have the same semantics
 - Example: fcc phase in steels can be referred to as fcc, austenite or γ .
- Ontology-based Data Integration
 - Using ontologies to unify data that share some common semantics but originate from unrelated sources
 - Example: Are property data from two experiments consistent enough to be combined?
- Ontologies are not static and can grow with needs

Ontologies & Graph Databases

The image shows two overlapping screenshots of the Neo4j web interface. The top screenshot displays a table of relationships for the query 'rels:193'. The bottom screenshot shows a graph visualization of the same data, with nodes and relationships represented as a network.

Relationship	Start node	Type	End node	source
Relationship 7218	Node 1976	domain	Node 193	"http://www.w3.org/2000/01/rdf-schema#domain"
Relationship 4207	Node 1196	domain	Node 193	"http://www.w3.org/2000/01/rdf-schema#domain"
Relationship 4189	Node 1190	domain	Node 193	"http://www.w3.org/2000/01/rdf-schema#domain"
Relationship 3992	Node 1125	domain	Node 193	"http://www.w3.org/2000/01/rdf-schema#domain"
Relationship 2722	Node 749	domain	Node 193	"http://www.w3.org/2000/01/rdf-schema#domain"
Relationship 2659	Node 729	domain	Node 193	"http://www.w3.org/2000/01/rdf-schema#domain"
Relationship 2391	Node 640	domain	Node 193	"http://www.w3.org/2000/01/rdf-schema#domain"

- Why use a graph database?
 - True networked database with queries, ACID, and REST interface
 - All apps can share the same representation
 - Overcomes some of the limitations of RDF
 - Flexible visualization...

UML Domain Model

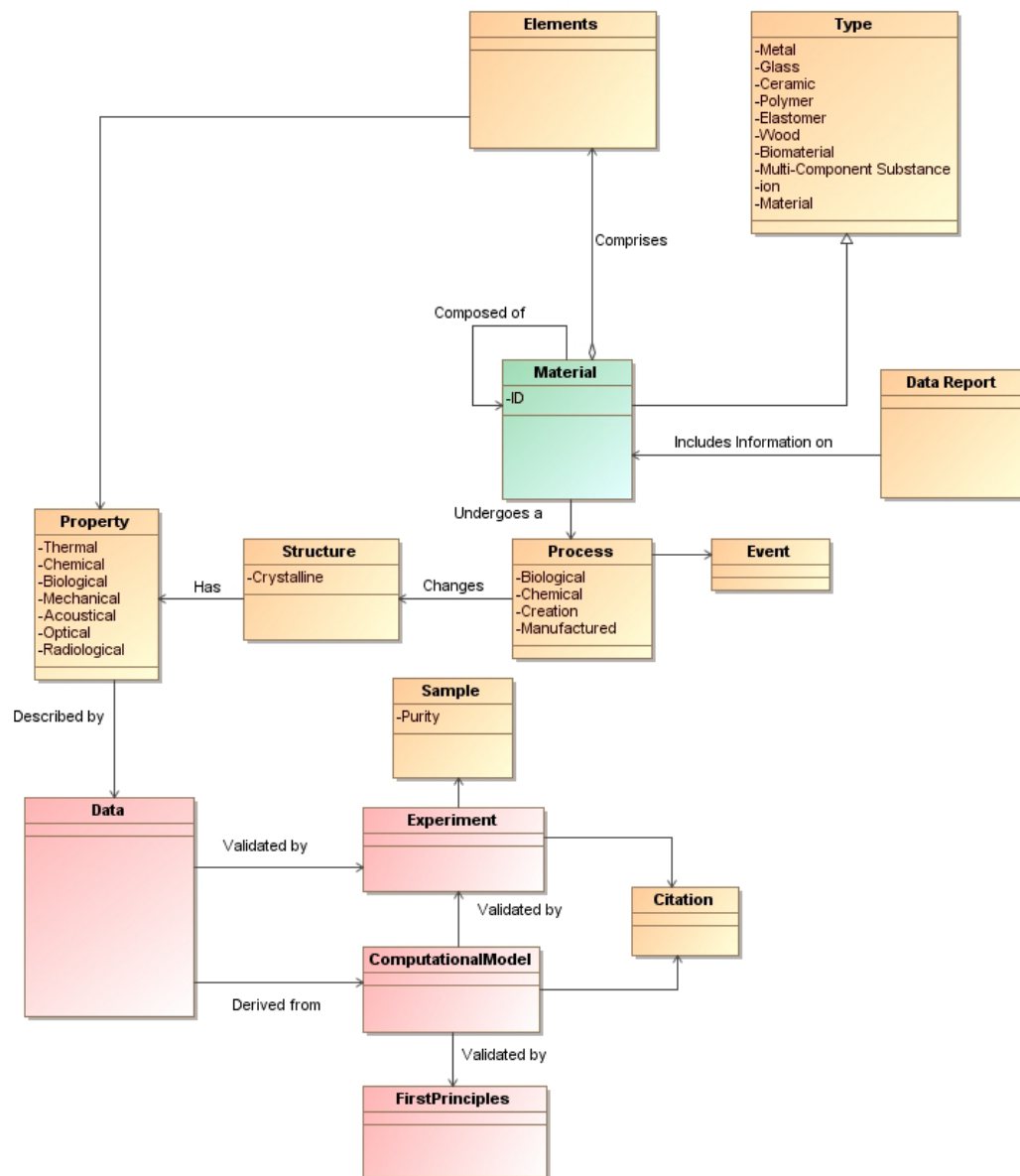
Sources

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

Tools

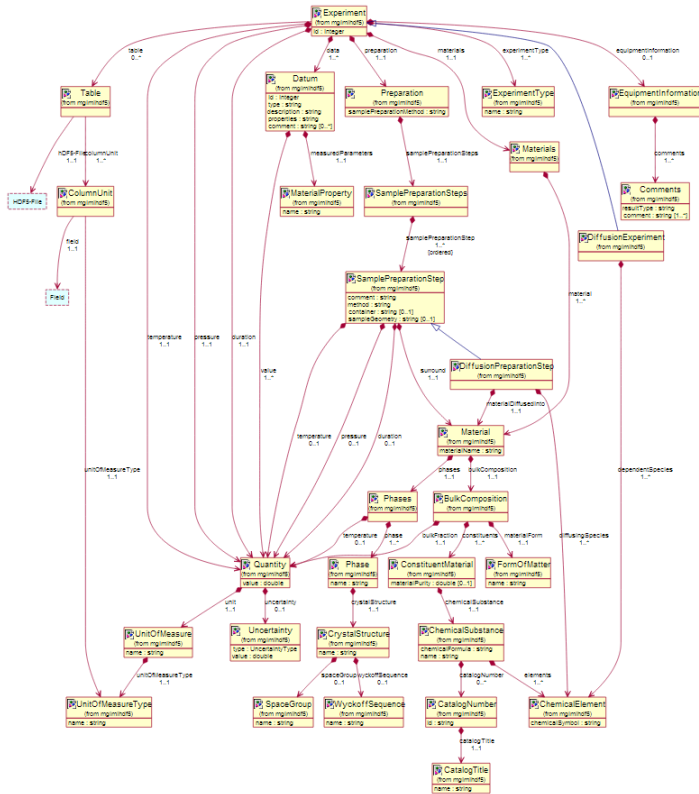
- UML (Unified Modeling Language)
- Semantic Web (RDF, OWL)

Note: This is a generalized model depicting overall structure

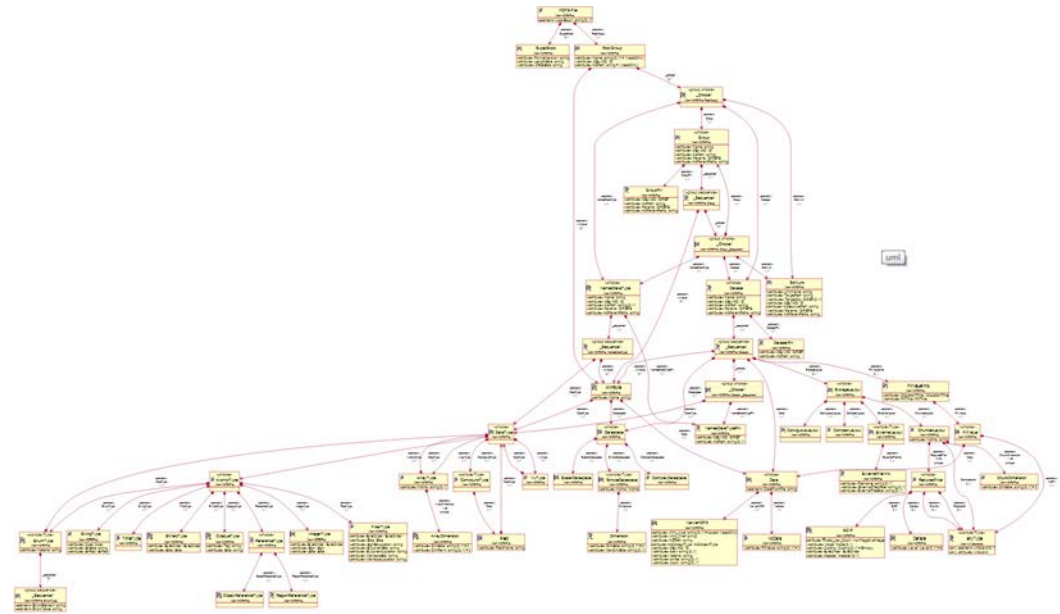


Encoding CALPHAD Data

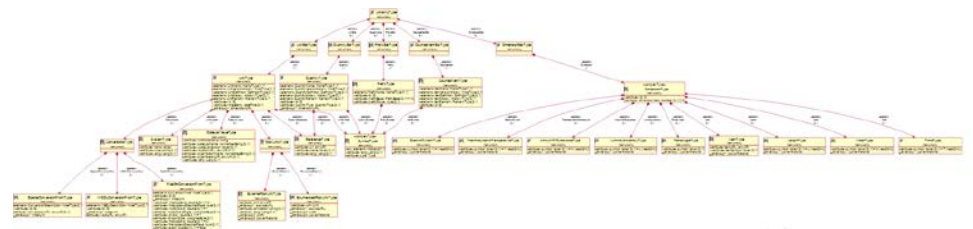
Core CALPHAD



Tabular Data (HDF5)



Measurement Units (Units ML)



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.



Experiment

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



Experiment

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



Experiment

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



Snap-Shot of XML Format

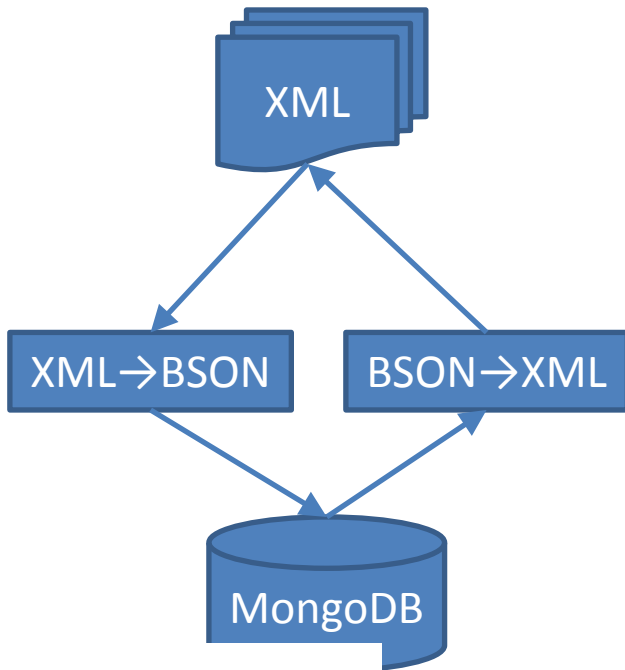
XML View

This is a preview of the XML which will be generated. Each modification you make in the form will be written in this preview.

```
<experiment xmlns:hdf5="http://hdfgroup.org/HDF5/XML/schema/HDF5-File">
  <experimentType>
    <tracerDiffusivity>
      <material>
        <materialName>
          Mg
        </materialName>
        <phase>
          <name>
            HCP
          </name>
          <crystalStructure>
            <spaceGroup>
              <symbolOrNumber />
            </spaceGroup>
            <wyckoffSequence>
              <sequence />
            </wyckoffSequence>
          </crystalStructure>
        </phase>
        <Composition>
          <quantityUnit>
            mass fraction
          </quantityUnit>
          <constituents>
```

- Why XML?
 - Internationalization
 - Flexibility
 - Transformability
 - Interoperability
 - Longevity
 - Web-Enabled
 - Available Resources

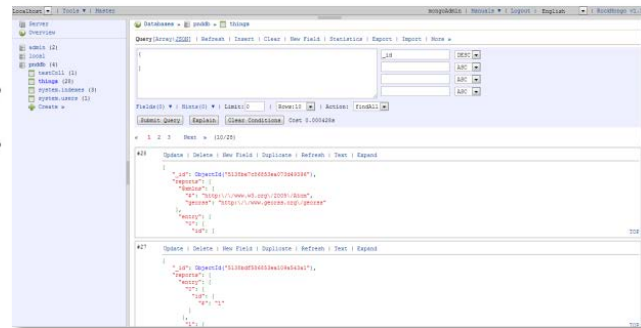
XML Document Storage



- MongoDB
 - Schema-less, cloud-friendly
 - High Performance, scalable
 - Used by CERN enable information discovery on Compact Muon Solenoid data

- Reason: “dynamic queries, full indexes, including inner objects and embedded arrays, as well as auto-sharing”

```
{
  "_id"      : ObjectId("4be97eabcd1b30e86000003"),
  "title"   : "Ordered List",
  "creator_id" : ObjectId("4be97eabcd1b30e86000001"),
  "memberships" : [
    ObjectId("4be97eabcd1b30e86000001"),
    ObjectId("4be97eabcd1b30e86000002")
  ]
}
```



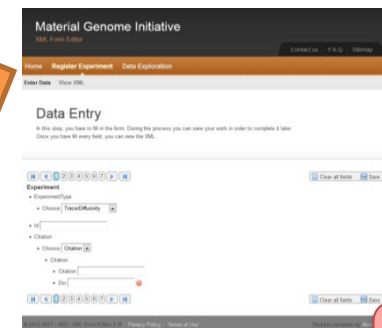
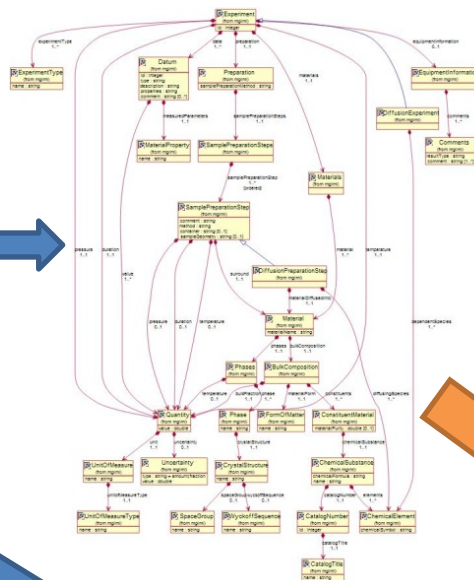
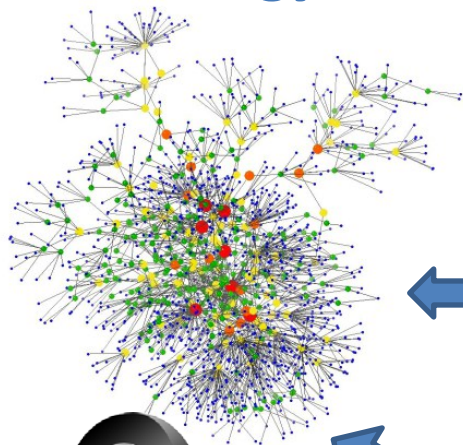
Future Data Informatics

User interface

Data Capture

Ontology

XML Schema



Data Tools:
Statistics; Machine Learning

Various Database Platforms

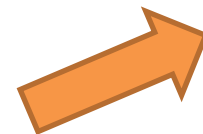
mongoDB

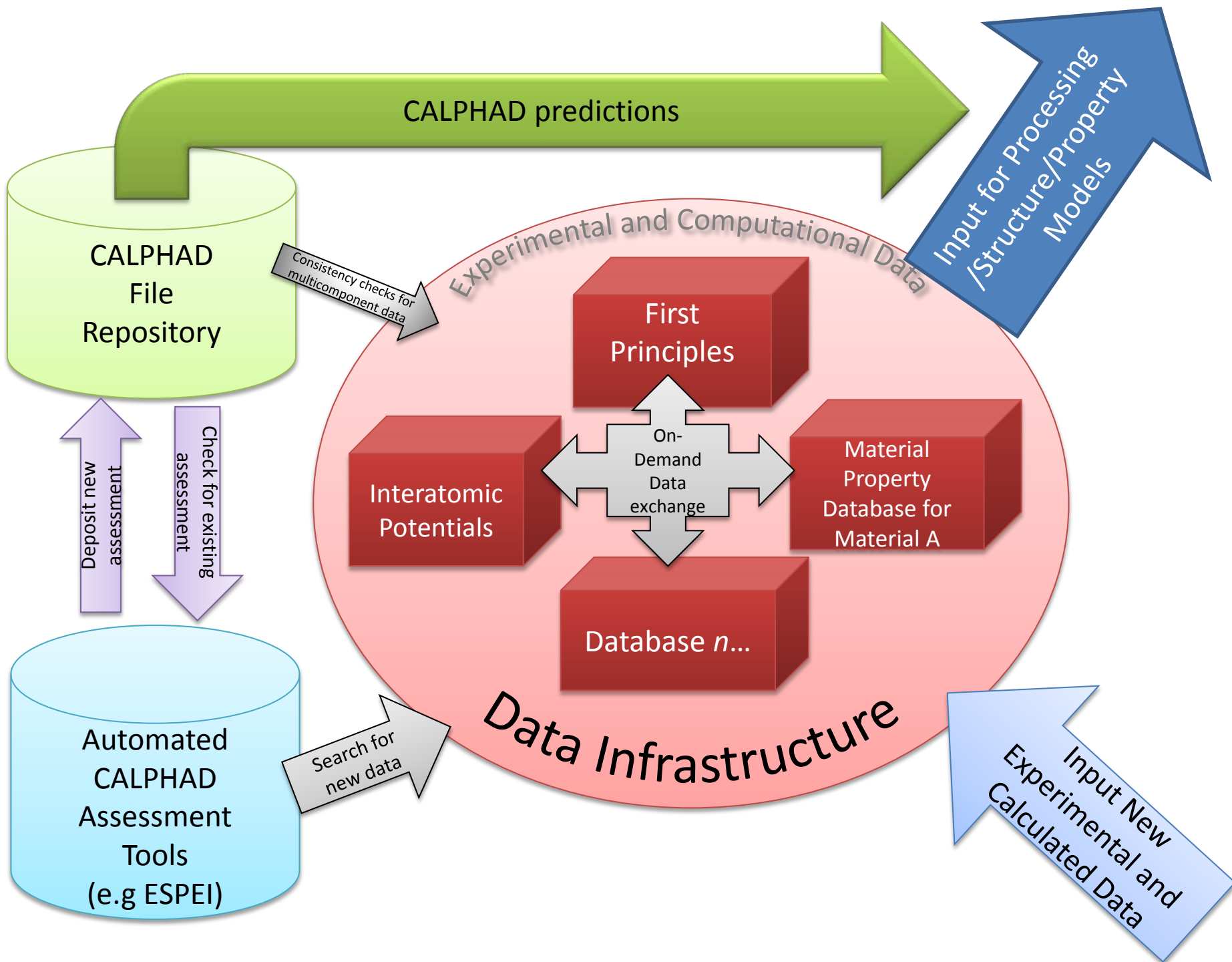
DSPACE

Neo4j
the graph database



UNIFIED MODELING LANGUAGE





Future: Needs Community Input

- **Need feedback on developing infrastructure**
- **Community needs to help define data standards (XML Schemas) – Long term benefit better data for everyone**
- **Willingness to share pre-competitive data and respect for data shared by others (need to reference contributed data)**

Want to know more: Attend the NIST Diffusion Workshop, May 9-10 at NIST



http://www.nist.gov/mml/msed/thermodynamics_kinetics/Diffusion-Workshop-Group.cfm

Extra slides on a test data schema for
tracer diffusivity

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.



Experiment

ExperimentType

Choose TracerDiffusivity

Id

Citation

Choose Citation

Citation

Citation

Doi



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



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



Example Entry

Data Entry

In this step, you have to fill in the form. During the process you can save your work in order to complete it later. Once you have fill every field, you can view the XML.



Experiment

- ExperimentType

- Choose

- Id

- Citation

- Choose

- Citation

- Citation

- Doi



Experiment

- ExperimentType
 - Choose **TracerDiffusivity**
 - TracerDiffusivity
 - Material
 - MaterialName **Mg**
 - Phase
 - Name **HCP_A3**
 - CrystalStructure
 - SpaceGroup
 - SymbolOrNumber **p63/mmc**
 - WyckoffSequence
 - Sequence
 - Composition
 - QuantityUnit **mass percent**
 - Constituents
 - Element **Mg**
 - Quantity **99.9**
 - Purity **99.9**
 - Error
 - MaterialForm
 - Choose **Polycrystalline**
 - Polycrystalline
 - AverageGrainSize **10**
 - Length **micrometer**

ExperimentType

- Choose **TracerDiffusivity**
 - TracerDiffusivity
 - DiffusingSpecies
 - Element **Mg**
 - MaterialPurity **99.999**
 - ExperimentalConditions
 - MeasurementConditions
 - Time
 - Duration **1000**
 - Unit **seconds**
 - Uncertainty
 - Type **amount**
 - Value
 - Temperature
 - Temperature **273**
 - Unit **Kelvin**
 - Uncertainty
 - Type **amount**
 - Value **1**
 - MeasurementConditions
 - Time
 - Duration **1000**
 - Unit **seconds**
 - Uncertainty
 - Type **amount**
 - Value
 - Temperature
 - Temperature **323**
 - Unit **Kelvin**
 - Uncertainty
 - Type **amount**
 - Value **1**
 - MeasurementConditions
 - Time
 - Duration **1000**
 - Unit **seconds**
 - Uncertainty
 - Type **amount**
 - Value
 - Temperature
 - Temperature **373**
 - Unit **Kelvin**
 - Uncertainty
 - Type **amount**
 - Value **1**

Enter the 3 temperatures at which the diffusivity was measured.



Experiment

- ExperimentType
 - Choose
 - TracerDiffusivity
 - SamplePreparations
 - SampleGeometry
 - Geometry
 - MaterialName
 - Geometry
 - Geometry
 - MaterialName
 - Geometry
 - SamplePreparationProcedure
 - ProcedureName
 - ProcedureDescription
 - SamplePreparationProcedure
 - ProcedureName
 - ProcedureDescription
 - SamplePreparationProcedure
 - ProcedureName
 - ProcedureDescription



Experiment

- ExperimentType
 - Choose
 - TracerDiffusivity
 - Measurement
 - Type
 - ExperimentalMethod
 - Choose
 - Direct
 - Choose
 - SIMS
 - SimsInstrument
 - PrimaryBeamSource
 - Energy
 - EnergyUnit
 - RasterArea
 -
 - DetectionArea
 - DetectionAreaUnit
 - DataCollectionMethod





Experiment

- ExperimentType

- Choose

- TracerDiffusivity

- MeasuredValues + -

- MeasurementDescription

- Value + -

- Choose

- Profile

Table module

+ -



- DataAnalysis

- DataAnalysisMethod + -

- Method + -

- Choose

- ArrheniusFit

- D0

- D0Unit

- Name

- UnitOfMeasureType

- Name

- Q

- QUnit

- Name

- UnitOfMeasureType

- Name

- MinTemperature

- Temperature

- Unit

- Uncertainty -

- Type

- Value

- MaxTemperature

- Temperature

- Unit

- Uncertainty -

- Type

- Value

- Description

- Results + -

- FileExtension

- Reference

