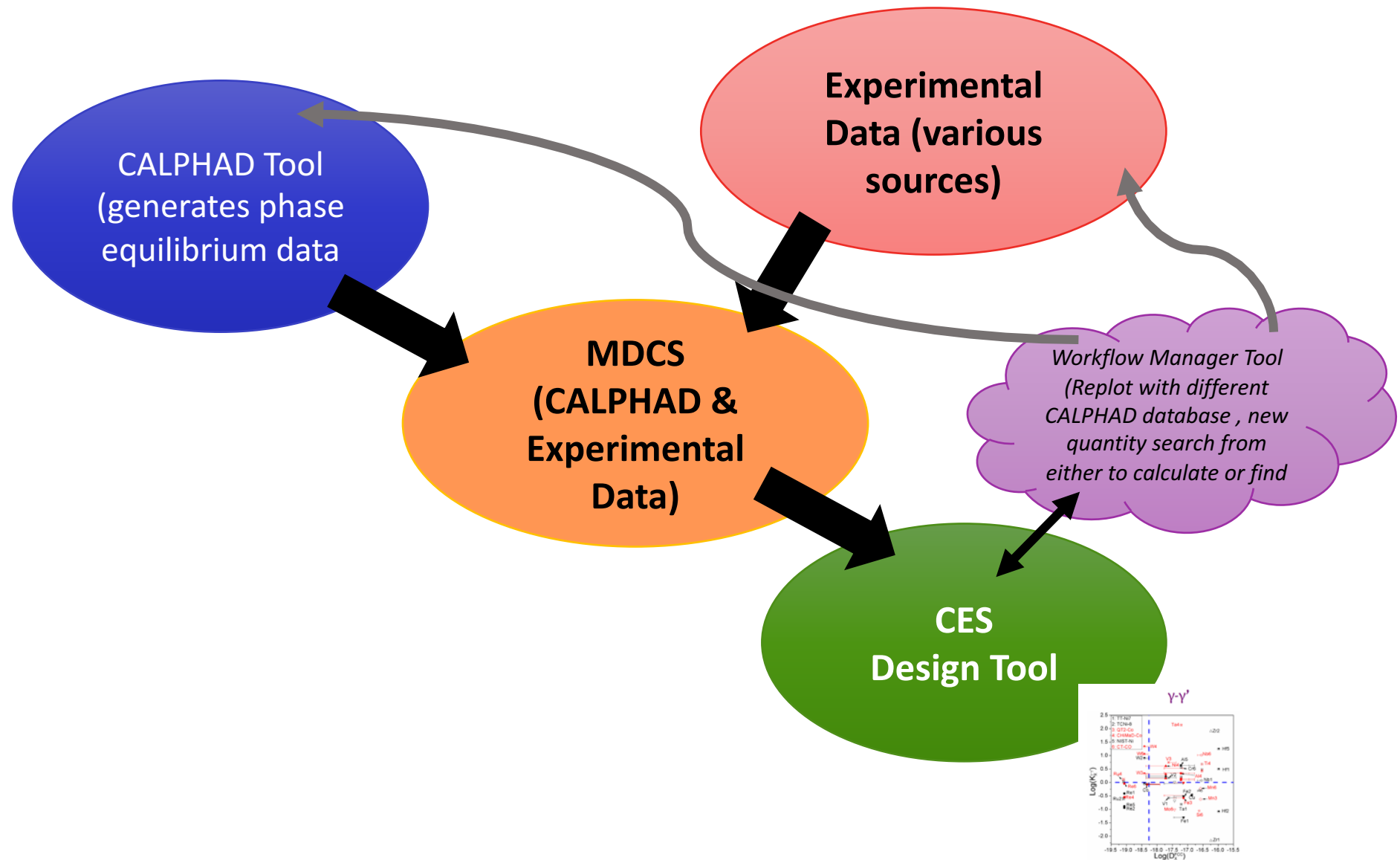


# Schemas Currently Developed or Being Developed

---

- Diffusion
  - Tracer/Impurity Diffusion Data in the Literature
  - Experimental Interdiffusion Data
- Phase Equilibria Data
  - Partitioning Coefficients (Co alloys) Shengyen Li
  - Ni-base superalloy data Shengyen Li /Questek
- Thermo Electrics (draft )
- ThermoML (NIST/TRC)
- Atom Probe Tomography (in progress)
- Polymers
  - Nanomine

# Possible Workflow



# Search for Data in MDCS

## Materials Data Curation System

Welcome, admin. Thanks for logging in.

Logout | Dashboard | Help

Home Data Curation Data Exploration Composer

Query by Example Search by Keyword OAI-PMH Search by Keyword

Refine by Template

Global Templates

- DiffusionDemo
- partitioningscreening
- interDiffusion

User Defined Templates

Create your own templates using the [Composer](#) and you will be able to use them from this section.

### Search by keyword

Enter keywords, or leave blank to

41 results

- [Y-FCCA1\\_LIQ](#) partitioningscreening
- [Al-FCCA1\\_FCCL12](#) partitioningscreening
- [Al-FCCA1\\_LIQ](#) partitioningscreening
- [Co-FCCA1\\_FCCL12](#) partitioningscreening
- [Cr-FCCA1\\_FCCL12](#) partitioningscreening
- [Cr-FCCA1\\_LIQ](#) partitioningscreening
- [Cu-FCCA1\\_FCCL12](#) partitioningscreening
- [Cu-FCCA1\\_LIQ](#) partitioningscreening
- [Fe-FCCA1\\_FCCL12](#) partitioningscreening
- [Fe-FCCA1\\_LIQ](#) partitioningscreening
- [Hf-FCCA1\\_FCCL12](#) partitioningscreening
- [Hf-FCCA1\\_LIQ](#) partitioningscreening
- [Mn-FCCA1\\_FCCL12](#) partitioningscreening
- [Mn-FCCA1\\_LIQ](#) partitioningscreening
- [Mo-FCCA1\\_FCCL12](#) partitioningscreening
- [Mo-FCCA1\\_LIQ](#) partitioningscreening
- [Nb-FCCA1\\_FCCL12](#) partitioningscreening
- [Nb-FCCA1\\_LIQ](#) partitioningscreening

Data Exploration Composer

Keyword OAI-PMH Search by Keyword

### Search by keyword

Search for results from  
QT2-Co database

QT2-CO \*

22 results

- [Al-FCCA1\\_FCCL12](#) partitioningscreening
- [Al-FCCA1\\_LIQ](#) partitioningscreening
- [Co-FCCA1\\_FCCL12](#) partitioningscreening
- [Cr-FCCA1\\_FCCL12](#) partitioningscreening
- [Cr-FCCA1\\_LIQ](#) partitioningscreening
- [Fe-FCCA1\\_FCCL12](#) partitioningscreening
- [Fe-FCCA1\\_LIQ](#) partitioningscreening
- [Hf-FCCA1\\_FCCL12](#) partitioningscreening
- [Mn-FCCA1\\_FCCL12](#) partitioningscreening
- [Mn-FCCA1\\_LIQ](#) partitioningscreening
- [Mo-FCCA1\\_FCCL12](#) partitioningscreening
- [Nb-FCCA1\\_FCCL12](#) partitioningscreening
- [Ni-FCCA1\\_FCCL12](#) partitioningscreening
- [Ni-FCCA1\\_LIQ](#) partitioningscreening
- [Re-FCCA1\\_FCCL12](#) partitioningscreening
- [Ta-FCCA1\\_FCCL12](#) partitioningscreening
- [Ti-FCCA1\\_FCCL12](#) partitioningscreening
- [Ti-FCCA1\\_LIQ](#) partitioningscreening
- [V-FCCA1\\_FCCL12](#) partitioningscreening
- [V-FCCA1\\_LIQ](#) partitioningscreening
- [W-FCCA1\\_FCCL12](#) partitioningscreening
- [W-FCCA1\\_LIQ](#) partitioningscreening

Keyword OAI-PMH Search by Keyword

### Search by keyword

Search for results at  
the solidus  
temperature

solidus \*

19 results

- [Al-FCCA1\\_LIQ](#) partitioningscreening
- [Cr-FCCA1\\_LIQ](#) partitioningscreening
- [Cu-FCCA1\\_LIQ](#) partitioningscreening
- [Fe-FCCA1\\_LIQ](#) partitioningscreening
- [Hf-FCCA1\\_LIQ](#) partitioningscreening
- [Mn-FCCA1\\_LIQ](#) partitioningscreening
- [Mo-FCCA1\\_LIQ](#) partitioningscreening
- [Nb-FCCA1\\_LIQ](#) partitioningscreening
- [Ni-FCCA1\\_LIQ](#) partitioningscreening
- [Pd-FCCA1\\_LIQ](#) partitioningscreening
- [Pt-FCCA1\\_LIQ](#) partitioningscreening
- [Re-FCCA1\\_LIQ](#) partitioningscreening
- [Ru-FCCA1\\_LIQ](#) partitioningscreening
- [Si-FCCA1\\_LIQ](#) partitioningscreening
- [Ta-FCCA1\\_LIQ](#) partitioningscreening
- [Ti-FCCA1\\_LIQ](#) partitioningscreening
- [V-FCCA1\\_LIQ](#) partitioningscreening
- [W-FCCA1\\_LIQ](#) partitioningscreening
- [Zr-FCCA1\\_LIQ](#) partitioningscreening

Home | Composer | Contact

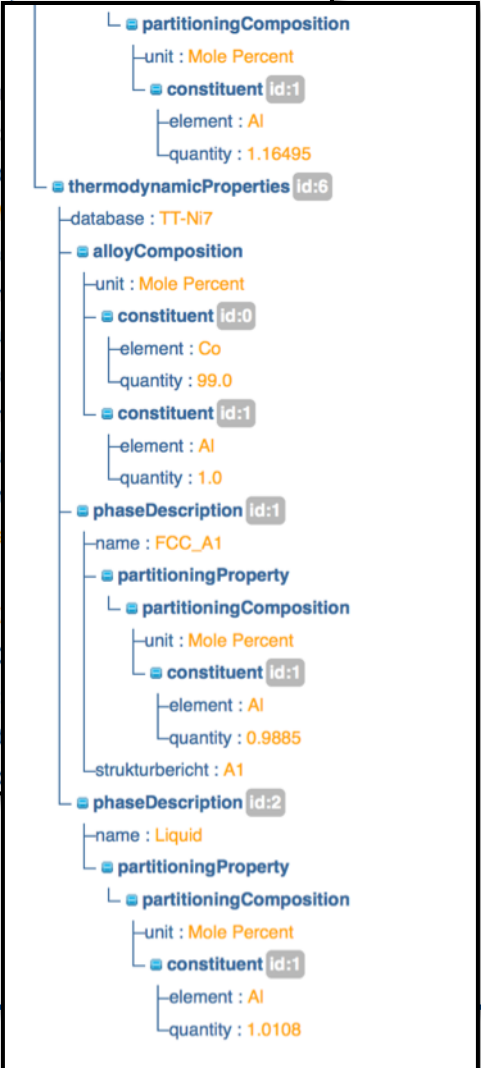
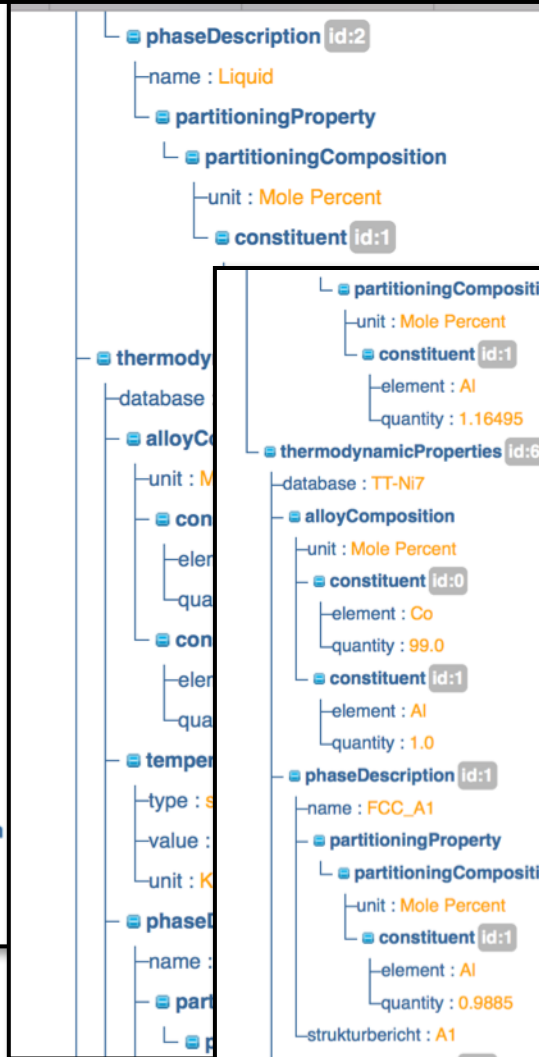
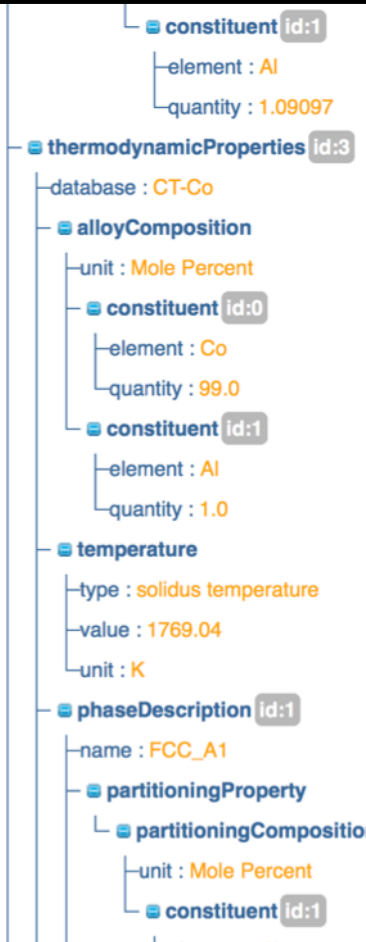
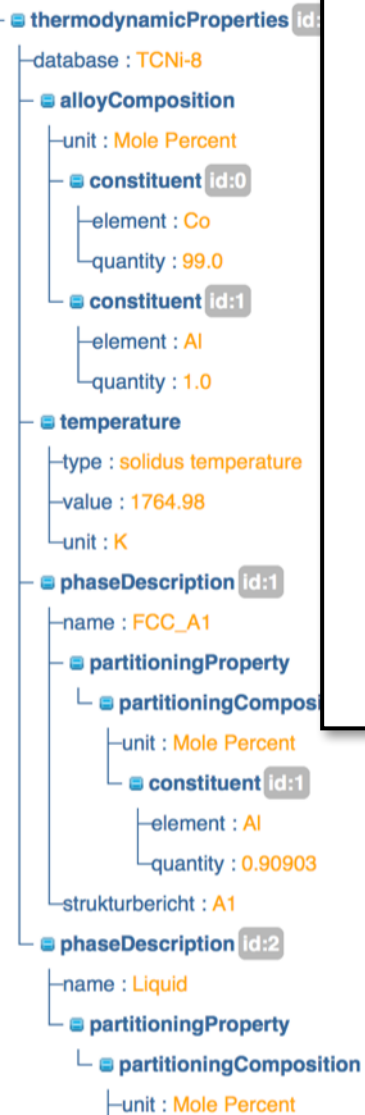
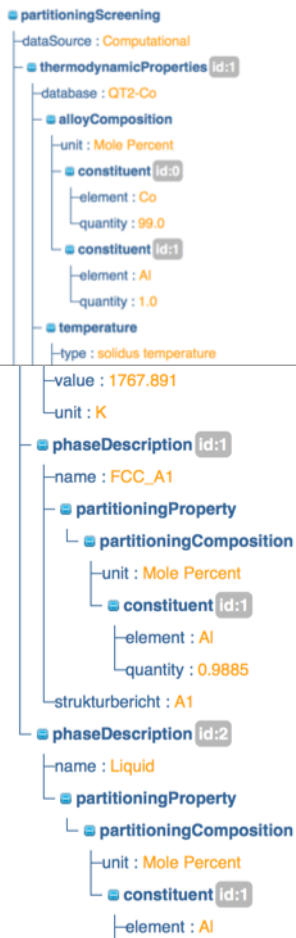
# Data Representation for AI Liquid Partitioning Behavior

Materials Data Curation System  
Welcome, admin. Thanks for logging in. Logout | D

Home Data Curation Data Exploration Composer

Query by Example Search by Keyword OAI-PMH Search by Keyword

## AI-FCCA1\_LIQ



# 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

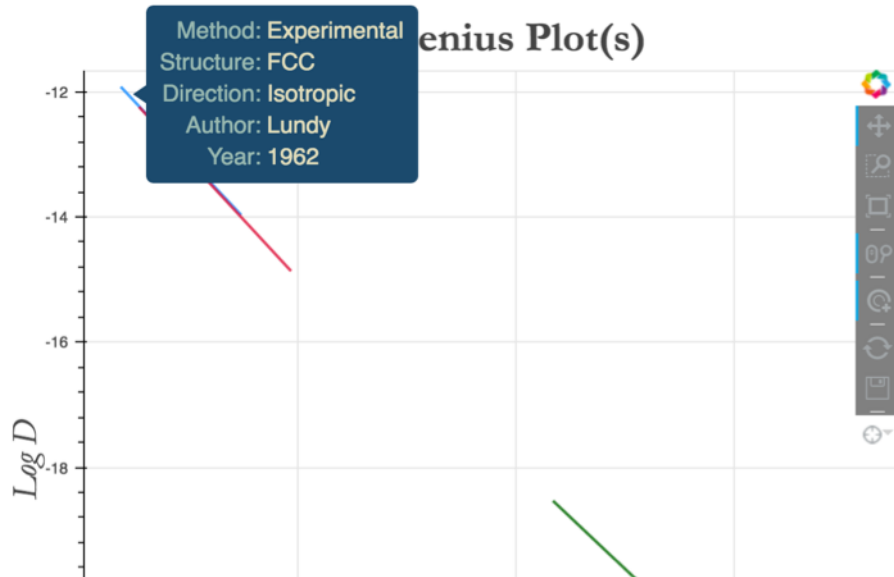
The screenshot displays the 'Materials Data Curation System' interface. At the top, there is a navigation bar with 'Home', 'Data Curation', 'Data Exploration', and 'Composer'. Below this, a sub-navigation bar shows 'Select Template', 'Enter Data', and 'View Data'. The main content area is titled 'Data Entry' and contains a form for entering data. The form is organized into sections: 'DiffusionCouple' (containing 'SampleId' with sub-fields for 'Id', 'SampleOwner', and 'Date'), and two 'Material' sections (each with sub-fields for 'MaterialName', 'NominalComposition', 'Phase', and 'AlloyForm'). At the top right of the form, there are buttons for 'Clear Fields', 'Save Form', and 'Download'. A sidebar on the left of the form area shows a progress indicator with three steps: '1 Select Template', '2 Enter Data' (the current step), and '3 View Data'.



# Linking Data

Method	Structure	Diffusion Direction	Frequency Factor D0 (m2/s)	Activation Energy Q (kJ/mole)	Temperature (K)	Details	Reference	Raw data
Experime...	fcc	isotropic	1.710e-04	142.4	729 - 916	26Al. Diffusion coup...	T.S. Lundy, J.F. Mur...	<a href="#">MDCS</a>
Experime...	fcc	isotropic	2.200e-04	144.4	673 - 883	26Al. Dried-on from...	M. Beveler, Y. Adda...	<a href="#">MDCS</a>
Experime...	fcc	isotropic	1.760e-05	126.5	358 - 482	Al. Void shrinkage (...)	T.E. Volin, R.W. Ball...	<a href="#">MDCS</a>
Experime...	fcc	isotropic	1.370e-05	123.6	515 - 770	Al. NMR. SLRT (27A...	R. Messer et al.: Pr...	<a href="#">MDCS</a>
First-prin...	fcc	isotropic	8.510e-04	131.2	654 - 934	DFT (PBEsol) + qua...	S.-L. Shang et al.: ...	not available
Experime...	fcc	isotropic	1.000e-05; 9.00e-04*	121.7; 172.8*	515 - 916	Al. NMR. SLRT (27A...	S. Dais, R. Messer. ...	not available
CALPHAD	fcc	isotropic	1.080e-05	126.7	300 - 900	Diffusion mobility m...	Y.W. Cui et al.: J. P...	not available
CALPHAD	fcc	isotropic	1.710e-04	142.0	300 - 900	Based on assessme...	A. Engstrom, J. Agre...	not available
CALPHAD	fcc	isotropic	8.233e-05	123.1	300 - 900	No details available	L. Zhang, Y. Du; NI...	not available
CALPHAD	hcp	⊥ c axis	2.380e-05	79.79	300 - 900	Estimation using th...	Y.W. Cui et al.: J. P...	not available

## Arrhenius Plot(s)



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

$$*D = D_0^1 \exp\left(\frac{-Q^1}{RT}\right) + D_0^2 \exp\left(\frac{-Q^2}{RT}\right)$$

$$**D = D_0 \exp\left(\frac{-Q}{RT}\right) \exp\left(\Omega \frac{(T_M)^2}{T^2}\right)$$

# Materials Data Curation System

Welcome, cecamp. Thanks for logging in.

Logout | My Profile | Help

Home | Data Curation | Data Exploration | Composer

Query by Example | Search by Keyword

## AlLundy1962.xml

### TracerDiffusivity

#### Citation

document-type : journal  
Title : Diffusion of Al26 and Mn54 in Aluminum  
author  
  GivenName : T. S.  
  Surname : Lundy  
author  
  GivenName : J. F.  
  Surname : Murdock  
PublicationName : Journal of Applied Physics  
publication-date  
  year : 1962  
volume : 33  
abstract : Diffusion coefficients of Al26 and Mn54 in aluminum have been determined for isotopes necessitated use of a thick layer technique. The exact solution to the problem in treating the data. Temperature dependence of the diffusion coefficients is given by  $D_{Mn54} = 0.22 \exp(-28800/RT)$  and  $D_{Al26} = 1.51 \exp(-14000/RT)$ .  
pages : 1671  
DOI : <http://dx.doi.org/10.1063/1.1728808>  
URL : <http://hdl.handle.net/11115/148>

#### Material

MaterialName : Al  
Phase  
  PhaseName : FCC  
  CrystalType  
    CrystalLattice : Cubic  
    structure : A1

### MeasuredValues

measurementDescription :  
MeasurementNote :  
DiffusionAxis : Isotropic  
value  
  profile  
    table  
      headers  
        column [id:0] : Source  
        column [id:1] : Material  
        column [id:2] : Exp  
        column [id:3] : Temp (K)  
        column [id:4] : 1/T  
        column [id:5] : D m2/s  
        column [id:6] : Error m2/s  
      rows  
        row [id:0]  
          column [id:0] : 62Lun  
          column [id:1] : sc  
          column [id:2] : Sec  
          column [id:3] : 916.51  
          column [id:4] : 10.91  
          column [id:5] : 1.22e-12  
          column [id:6] : 1.22e-13  
        row [id:1]  
          column [id:0] : 62Lun  
          column [id:1] : sc  
          column [id:2] : Sec  
          column [id:3] : 915.25  
          column [id:4] : 10.93  
          column [id:5] : 1.51e-12  
          column [id:6] : 1.51e-13  
        row [id:2]  
          column [id:0] : 62Lun  
          column [id:1] : sc  
          column [id:2] : Sec  
          column [id:3] : 895.42  
          column [id:4] : 11.17  
          column [id:5] : 8.55e-13  
          column [id:6] : 8.55e-14  
        row [id:3]

### DataAnalysis

#### arrheniusAnalysis

##### TemperatureRange

###### UpperTemperature

temperature : 916

unit : Kelvin

###### uncertainty

type : amount

value : 2

###### LowerTemperature

temperature : 723

unit : Kelvin

###### uncertainty

type : amount

value : 2

##### ActivationEnergy

EnergyValue : 142.4

Units : kJ/mole

##### PreExponentialCoefficient

D0\_Value : 0.000171

D0\_Units : m2/s



# Diffusion Data So Far

The screenshot shows a web browser window with the address bar displaying '127.0.0.1'. The main heading is 'Search by keyword'. On the left, there is a sidebar titled 'Refine by Template' with two sections: 'Global Templates' and 'User Defined Templates'. The 'Global Templates' section includes: demo-simple-file-upload, demo-simple-spreadsheet, DiffusionDemo, TracerDiffusion, TracerDiffusivity2, TracerDiffusivityMod, TracerDiffusivityMod2, TracerImpurity-Lit, and Interdiffusion-Exo. The 'User Defined Templates' section includes: Test-micrograph, test, and SEM-Image. The search bar contains the text 'Diffusion' and has a search icon. An 'Export' button is located to the right of the search bar. Below the search bar, it says '19 results ( Select/Unselect all)'. The results list consists of 19 entries, each with a checkbox, a plus icon, a filename, a template name, and a red 'X' icon. The entries are: Ni-Bakker1968.xml (TracerImpurity-Lit), Ni-Monma-1964.xml (TracerImpurity-Lit), Ni-Hirano-1961.xml (TracerImpurity-Lit), Ni-Messener-1961.xml (TracerImpurity-Lit), Ni-MacEwan2-1959.xml (TracerImpurity-Lit), Ni-Hoffman-1956.xml (TracerImpurity-Lit), Ni-Reyonlds-1957.xml (TracerImpurity-Lit), Au-Impurity-Al-Peterson1970.xml (TracerImpurity-Lit), Al-Impurity-Peterson1970.xml (TracerDiffusivityMod2), CoW-1000C.xml (Interdiffusion-Exo), CoW-test.xml (Interdiffusion-Exo), Al-Stoebe-1965.xml (TracerImpurity-Lit), Al-Burke-1972.xml (TracerImpurity-Lit), Al-Volin-1968.xml (TracerDiffusivityMod2), AlFradin-1967.xml (TracerDiffusivityMod), ALundy1962.xml (TracerDiffusivityMod), AlBeyeler1968.xml (TracerDiffusivity2), Al-Messer-1974.xml (TracerDiffusivityMod), and GE-DiffusionCouple-IN718-R95.xml (DiffusionDemo). The footer contains navigation links: Home | Data Curation | Data Exploration | Composer | Contact, and a 'Top ^' link.

Refine by Template

Global Templates

- demo-simple-file-upload
- demo-simple-spreadsheet
- DiffusionDemo
- TracerDiffusion
- TracerDiffusivity2
- TracerDiffusivityMod
- TracerDiffusivityMod2
- TracerImpurity-Lit
- Interdiffusion-Exo

User Defined Templates

- Test-micrograph
- test
- SEM-Image

## Search by keyword

Diffusion

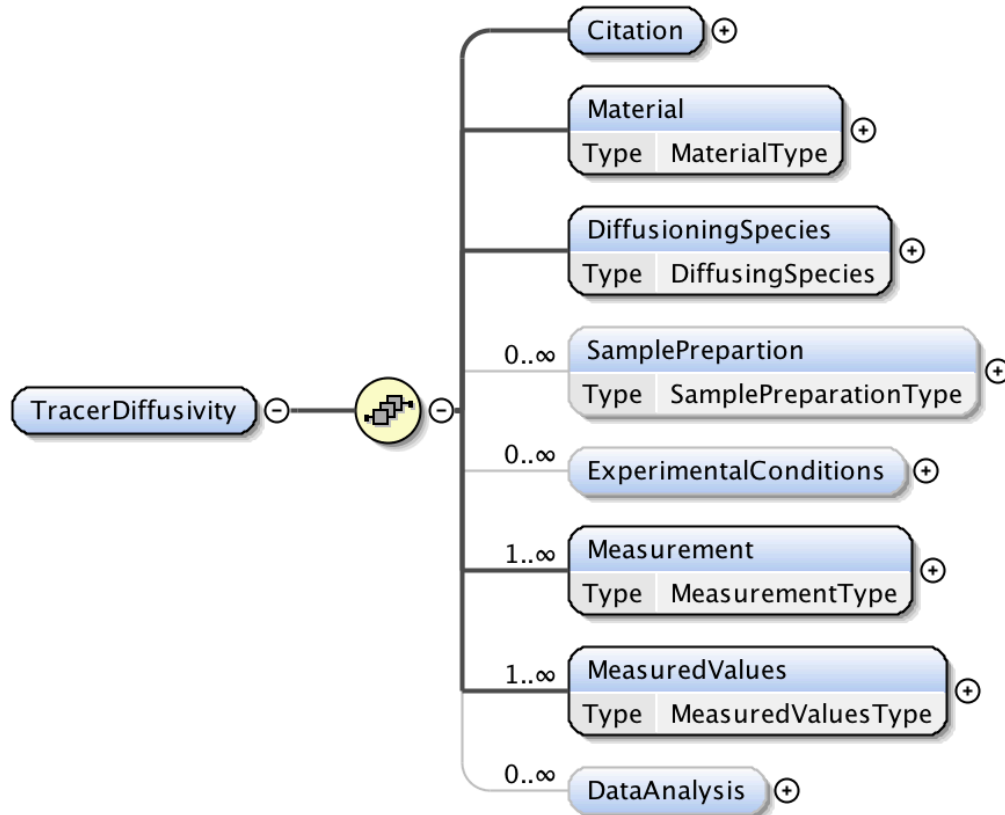
↓ Export

19 results (  Select/Unselect all)

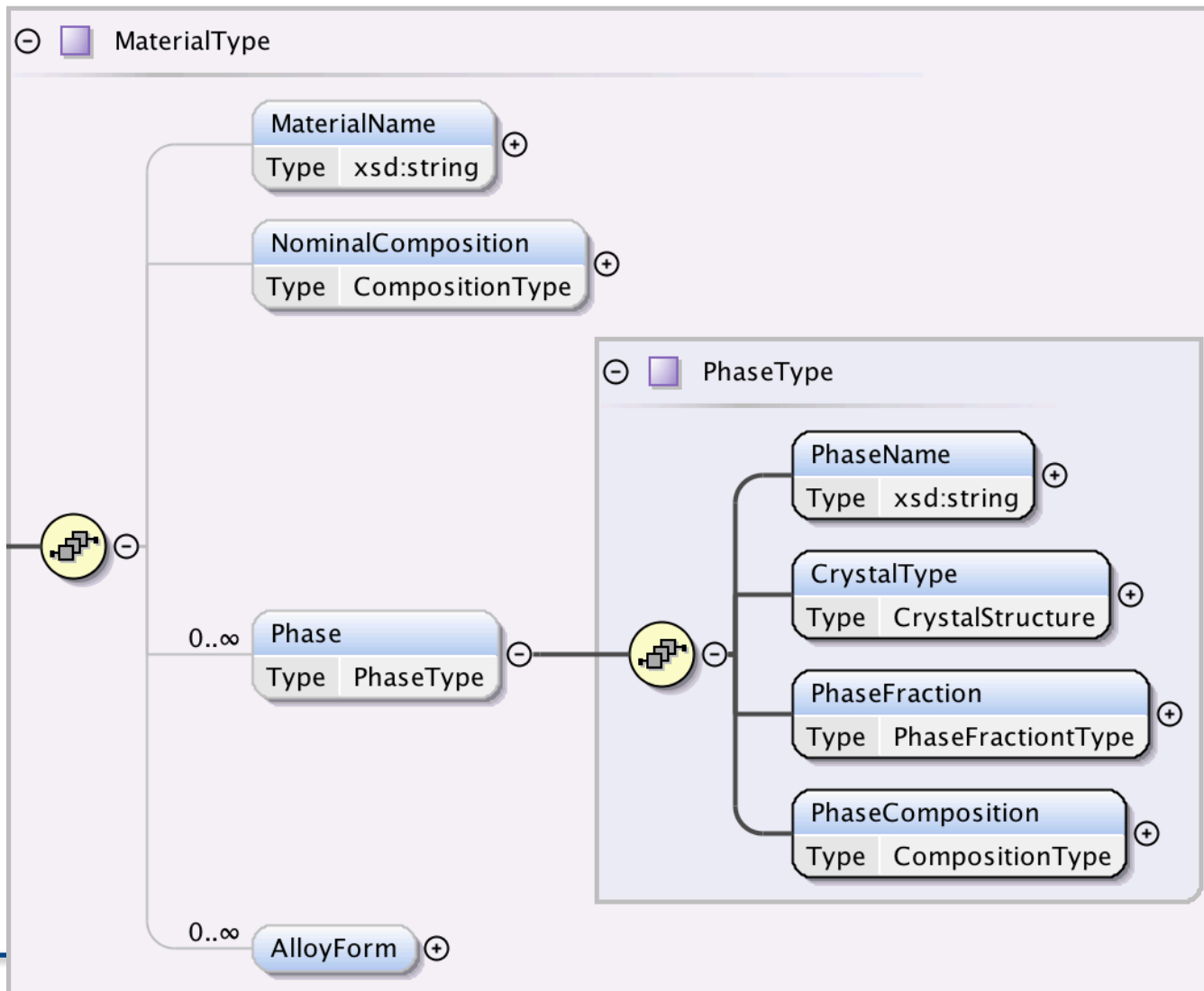
- [Ni-Bakker1968.xml](#) TracerImpurity-Lit
- [Ni-Monma-1964.xml](#) TracerImpurity-Lit
- [Ni-Hirano-1961.xml](#) TracerImpurity-Lit
- [Ni-Messener-1961.xml](#) TracerImpurity-Lit
- [Ni-MacEwan2-1959.xml](#) TracerImpurity-Lit
- [Ni-Hoffman-1956.xml](#) TracerImpurity-Lit
- [Ni-Reyonlds-1957.xml](#) TracerImpurity-Lit
- [Au-Impurity-Al-Peterson1970.xml](#) TracerImpurity-Lit
- [Al-Impurity-Peterson1970.xml](#) TracerDiffusivityMod2
- [CoW-1000C.xml](#) Interdiffusion-Exo
- [CoW-test.xml](#) Interdiffusion-Exo
- [Al-Stoebe-1965.xml](#) TracerImpurity-Lit
- [Al-Burke-1972.xml](#) TracerImpurity-Lit
- [Al-Volin-1968.xml](#) TracerDiffusivityMod2
- [AlFradin-1967.xml](#) TracerDiffusivityMod
- [ALundy1962.xml](#) TracerDiffusivityMod
- [AlBeyeler1968.xml](#) TracerDiffusivity2
- [Al-Messer-1974.xml](#) TracerDiffusivityMod
- [GE-DiffusionCouple-IN718-R95.xml](#) DiffusionDemo

Home | Data Curation | Data Exploration | Composer | Contact Top ^

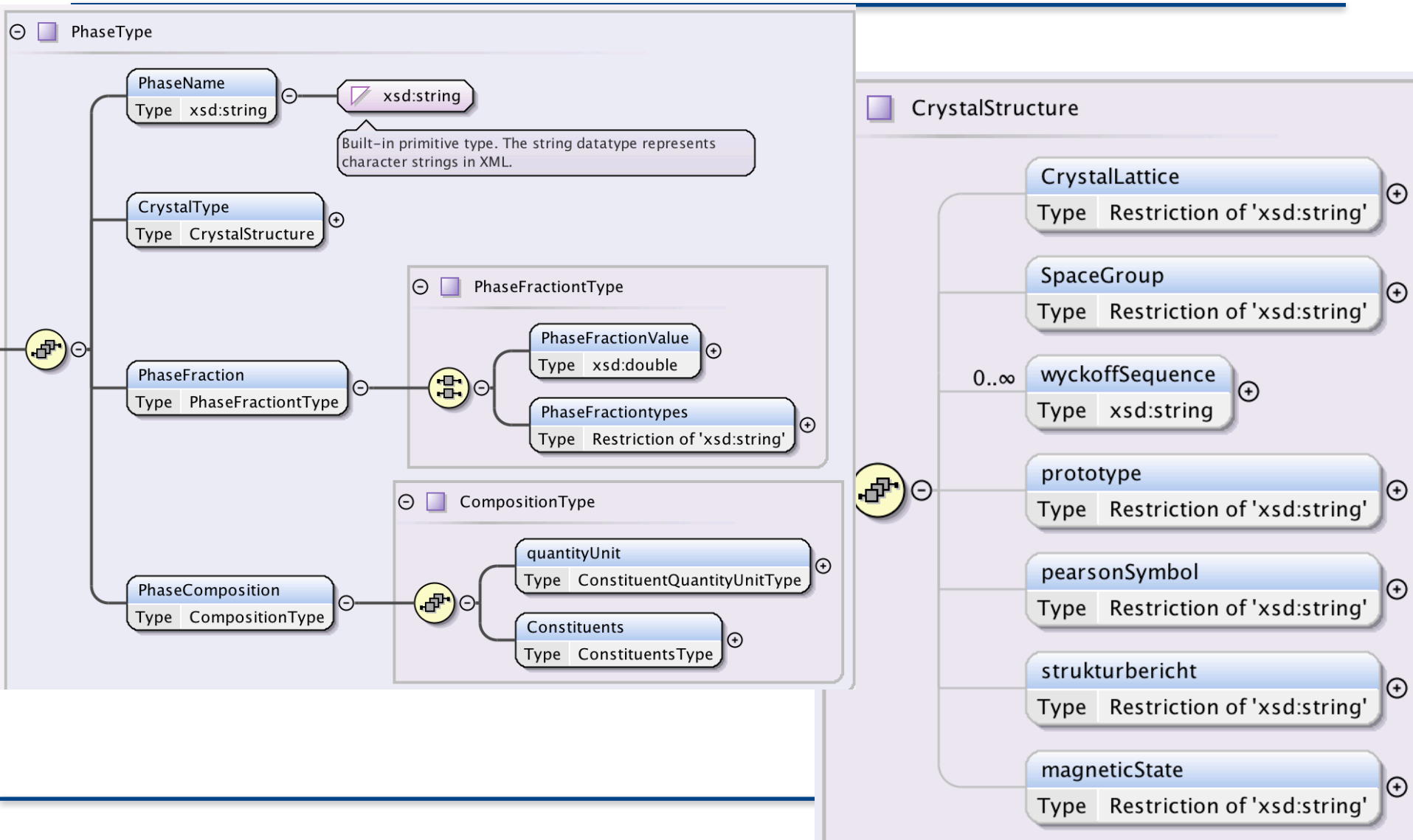
# Tracer/Impurity Diffusion Literature



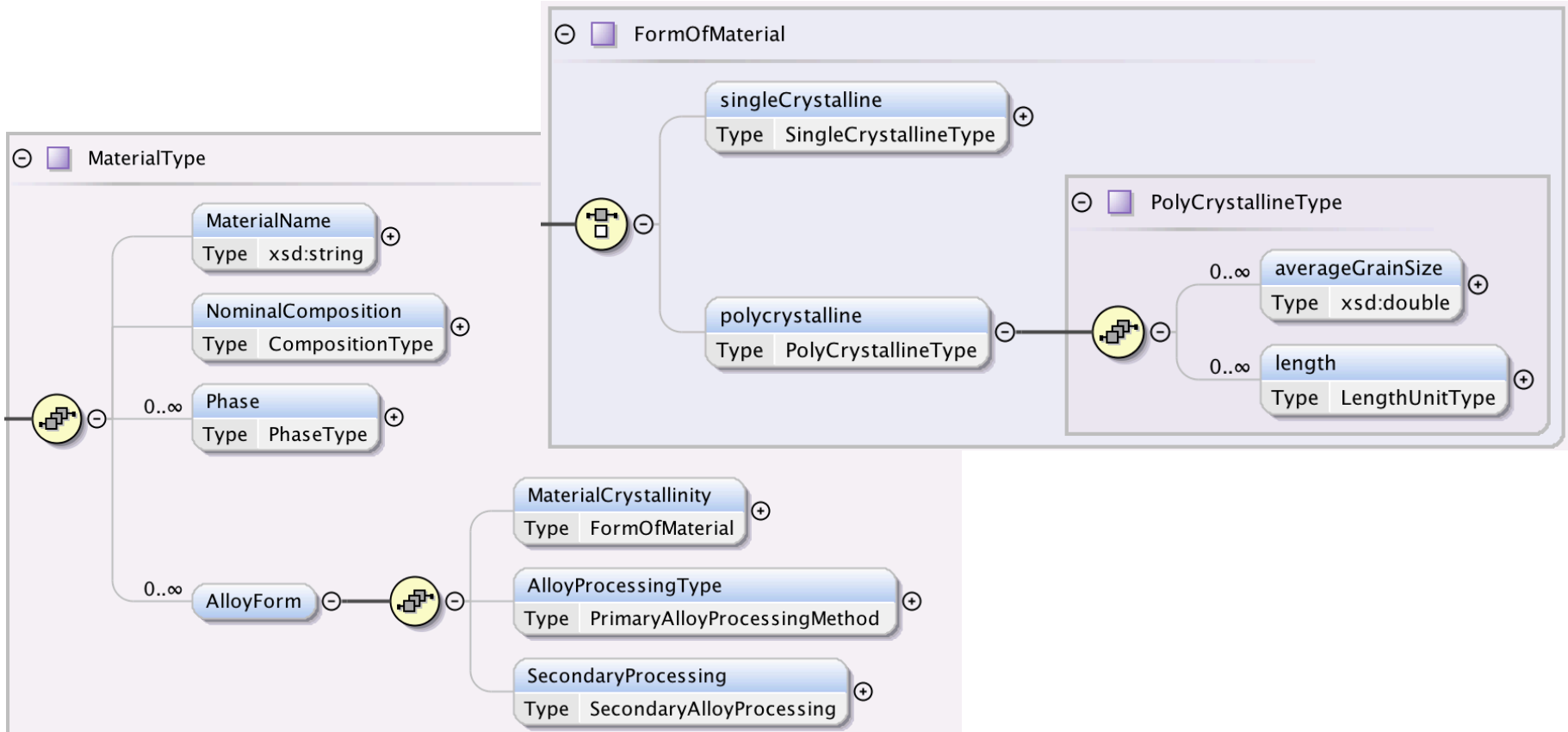
# Material Description

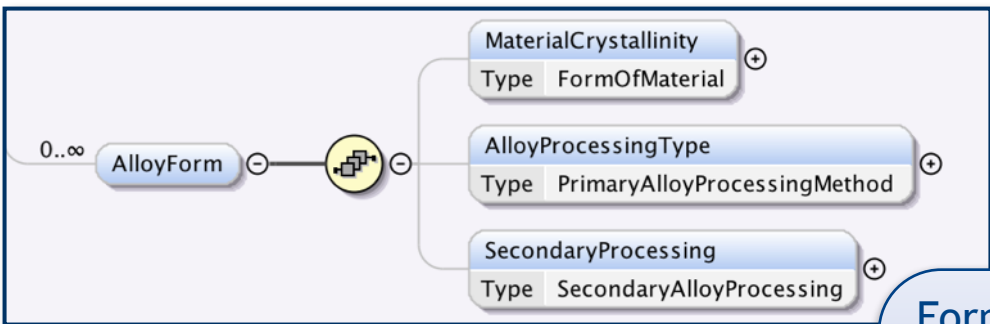


# Material/Phase Type and Crystal Structure



# Alloy Form

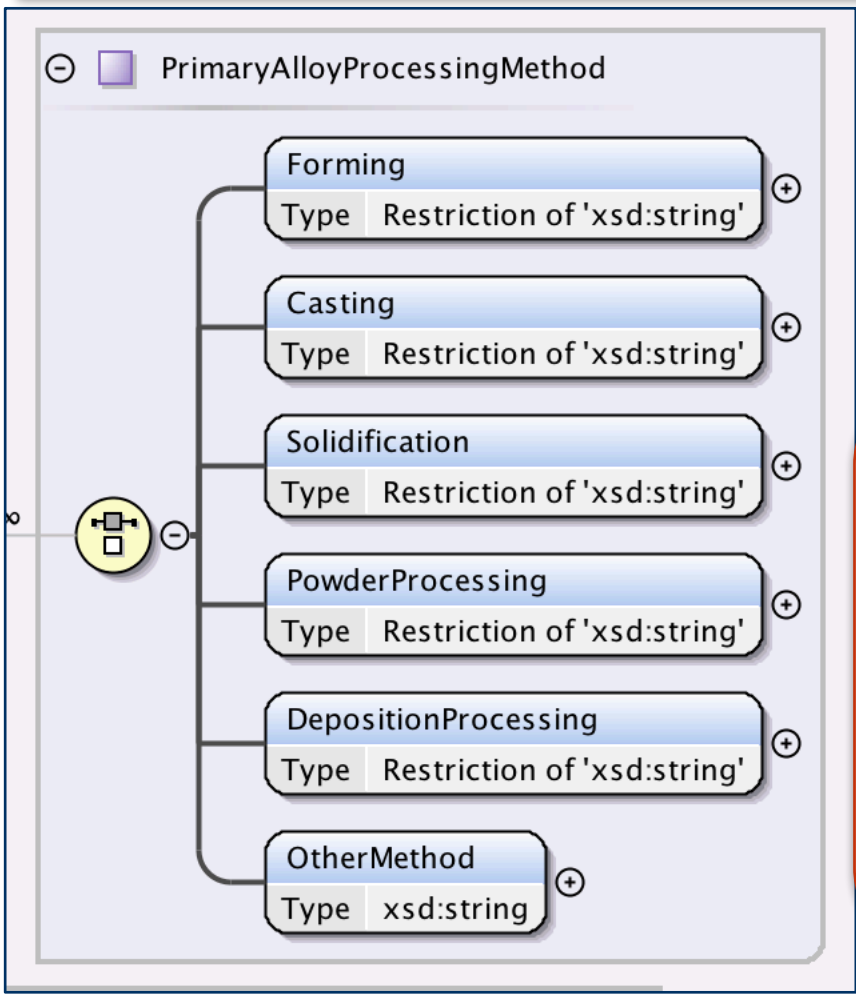




- ### Powder Processing
- Atomization
  - Ball Milling
  - Sponge Iron Process
  - Centrifugal Disintegration

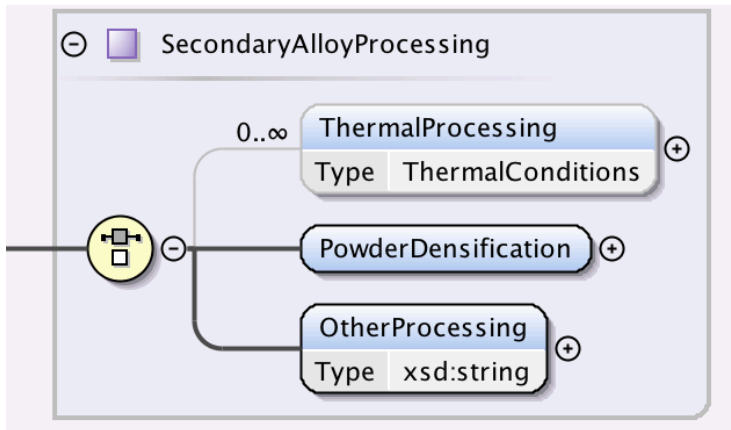
- ### Forming
- Forging
  - Cold Rolling
  - Hot Rolling
  - Extrusion
  - Drawing
  - Milling

- ### Casting
- Sand casting
  - Die casting
  - Investing casting
  - Slip casting
  - Continuous casting
  - Centrifugal casting
  - Vacuum arc melting



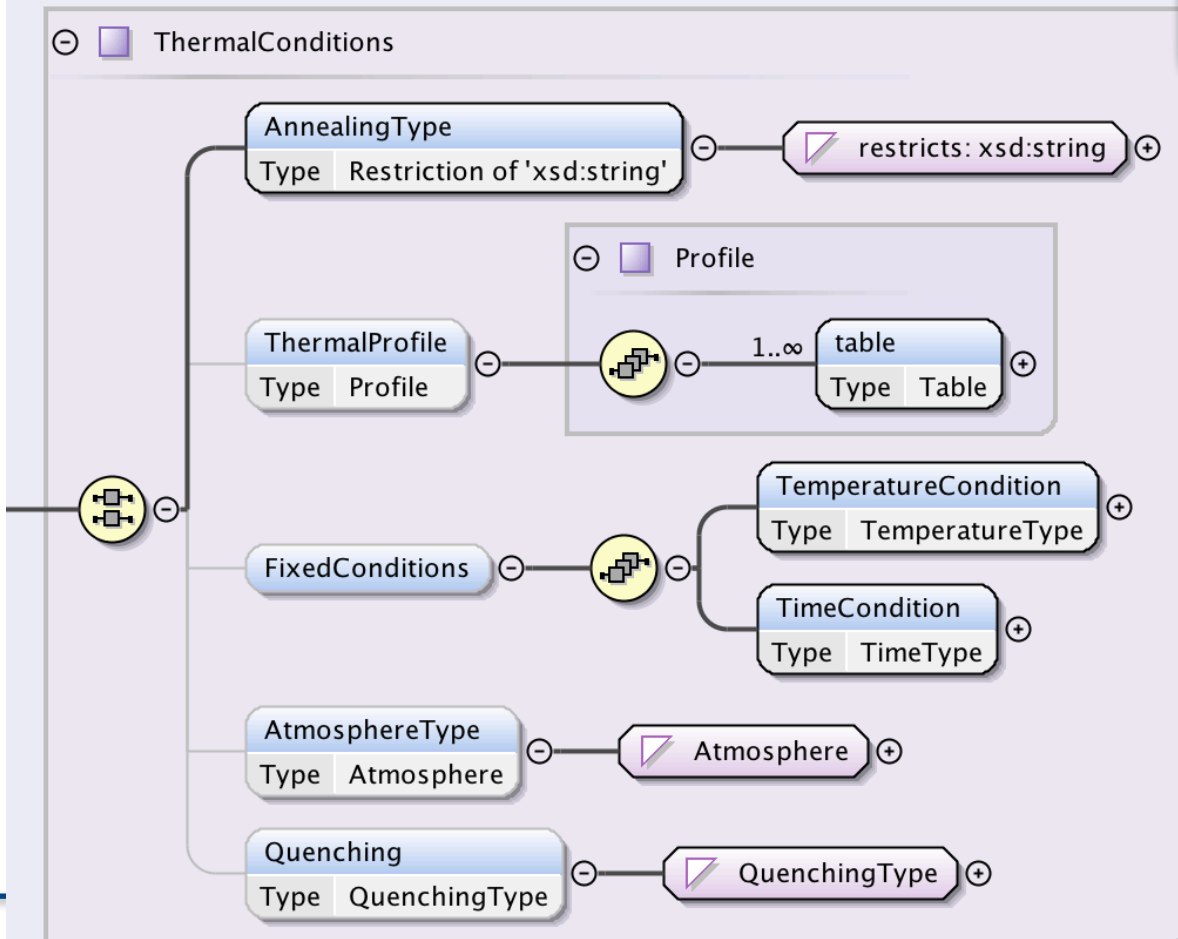
- ### Solidification
- Seeded Solidification
  - Directional Solidification
  - Zone Refining
  - Single Crystal Solidification
  - Rapid Solidification

- ### Deposition Processing
- Physical Vapor Deposition
  - Chemical Vapor Deposition
  - Sputter Coating
  - Electron Beam Deposition
  - Ion Beam Deposition
  - Plasma Spraying



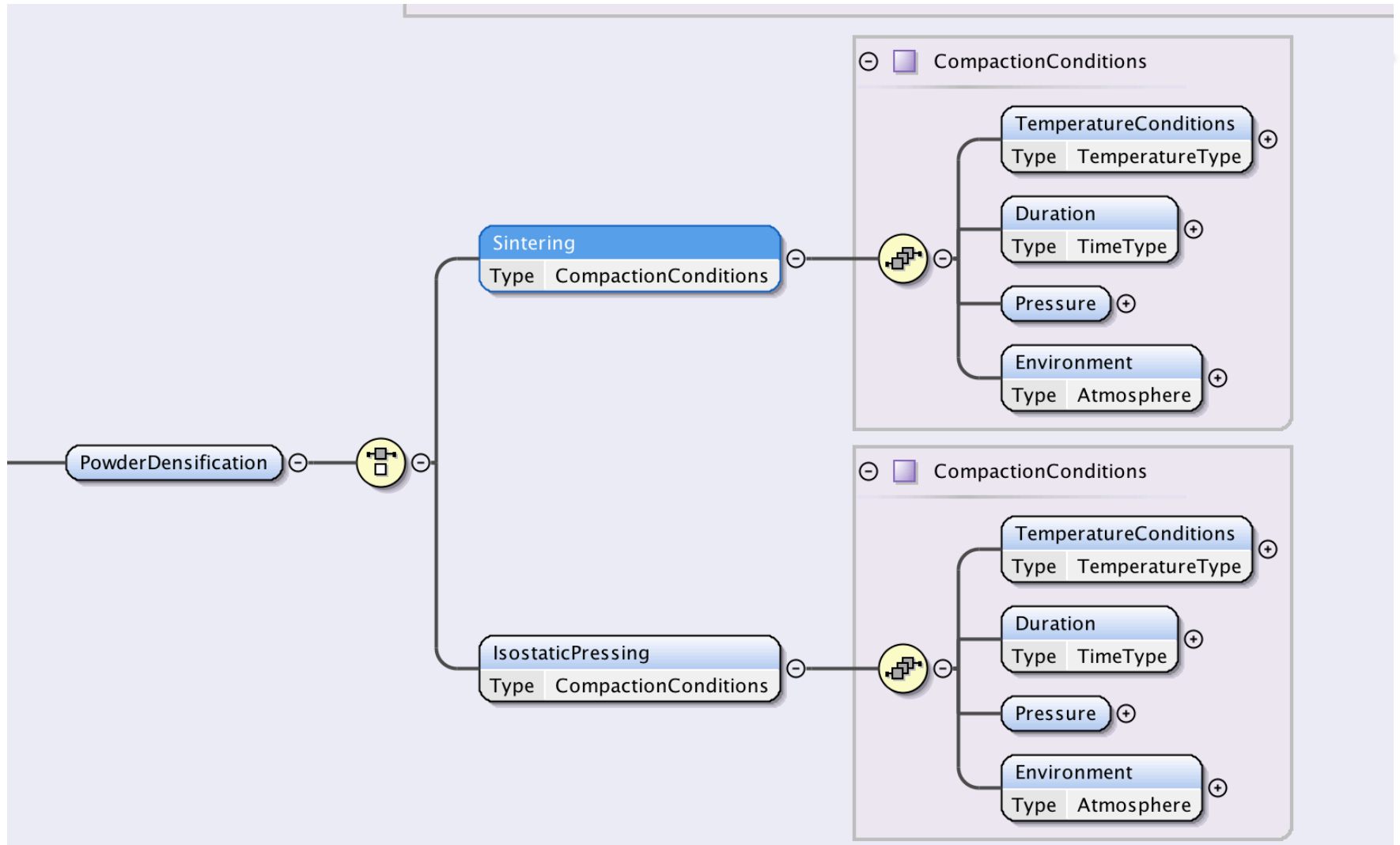
## Annealing Type

- Annealing
- Homogenization
- Aging
- Recrystallization
- Tempering
- Normalizing
- Stress Relieving
- Other



## Quenching Type

- Ice quench
- Water quench
- Brine quench
- Air cooled/quench
- Oil quench
- Furnace cooled
- Gas cooled
- Liquid N2 Quench







# NOMAD Meta Info

Search by name or description

Select Parent Section

Select Abstract Type

Select Type

number\_of\_basis\_functions\_in\_basis\_set\_atom\_centered  
 number\_of\_gaussian\_basis\_group\_contractio  
 ns  
 number\_of\_gaussian\_basis\_group\_exponents  
 number\_of\_kinds\_in\_basis\_set\_atom\_centere  
 d

## number\_of\_basis\_functions\_in\_basis\_set\_atom\_centered

**Type:** Dimension  
**Description:** Number of different basis functions in this [section\\_basis\\_set\\_atom\\_centered](#) . This equals the number of actual coefficients that are specified when using this basis set.

**Data Type:** i (integer value)

**Shape:** []

- Section
- Abstract Type
- Concrete Value
- Dimension

Disable zoom and panning  
 Reset view

- Section
- Abstract Type
- Concrete Value
- Dimension

Disable zoom and panning    Reset view



section\_basis\_set\_atom\_centered direct children:

- basis\_set\_atom\_centered\_ls
- basis\_set\_atom\_centered\_radial\_functions
- basis\_set\_atom\_centered\_short\_name
- basis\_set\_atom\_centered\_unique\_name
- basis\_set\_atom\_number
- number\_of\_basis\_functions\_in\_basis\_set\_atom\_centered
- number\_of\_kinds\_in\_basis\_set\_atom\_centered

## Ancestors

### Explicit Parents

[basis\\_set\\_description](#)

### Direct Children

[basis\\_set\\_atom\\_centered\\_short\\_name](#)  
[basis\\_set\\_atom\\_centered\\_unique\\_name](#)  
[basis\\_set\\_atom\\_centered\\_ls](#)  
[number\\_of\\_basis\\_functions\\_in\\_basis\\_set\\_atom\\_centered](#)  
[basis\\_set\\_atom\\_centered\\_radial\\_functions](#)  
[section\\_gaussian\\_basis\\_group](#)  
[section\\_basis\\_functions\\_atom\\_centered](#)  
[number\\_of\\_kinds\\_in\\_basis\\_set\\_atom\\_centered](#)  
[basis\\_set\\_atom\\_number](#)