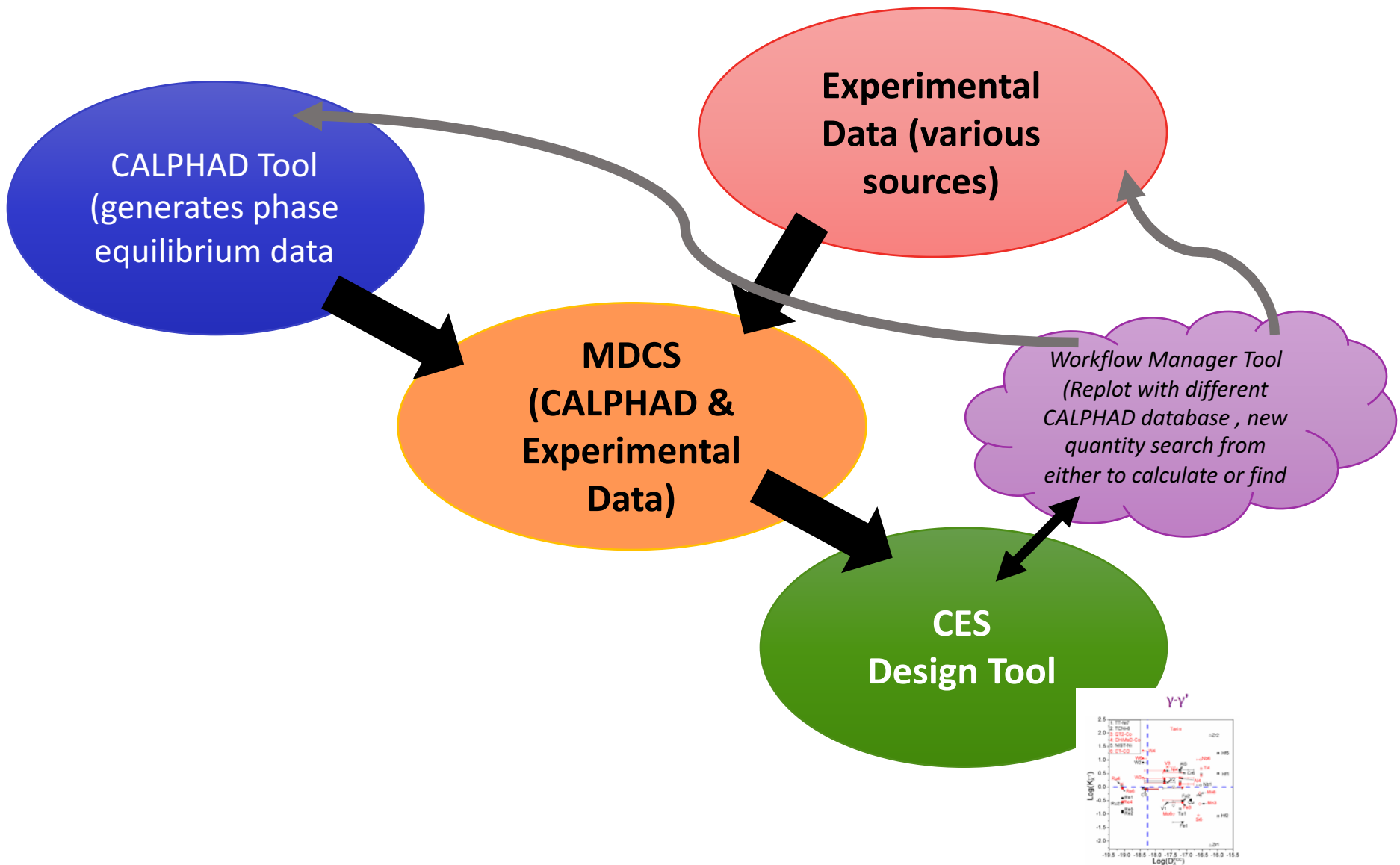


Schemas Currently Developed or Being Developed

- 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

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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

ion | Composer | Contact

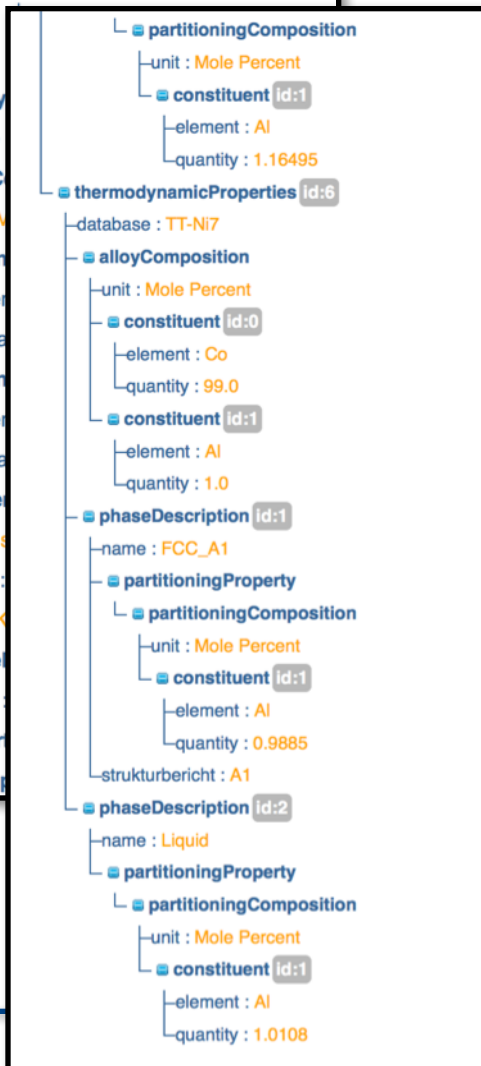
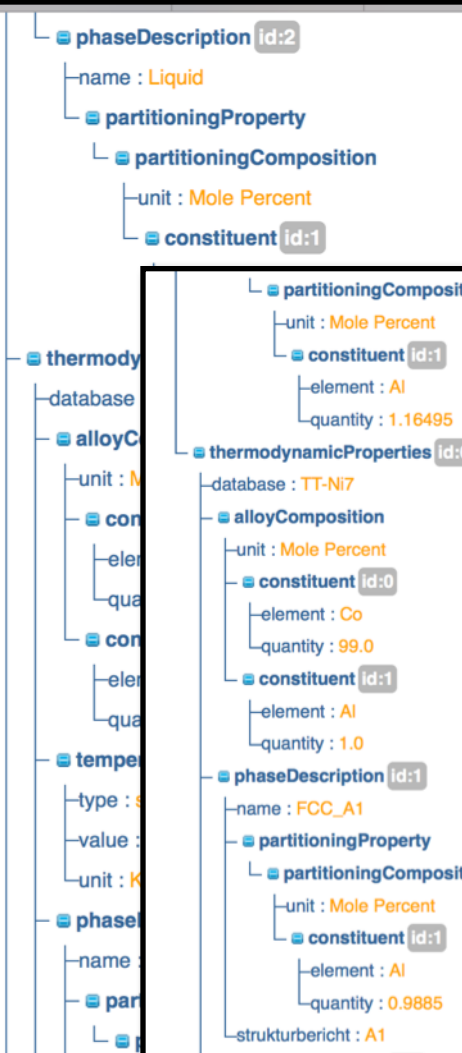
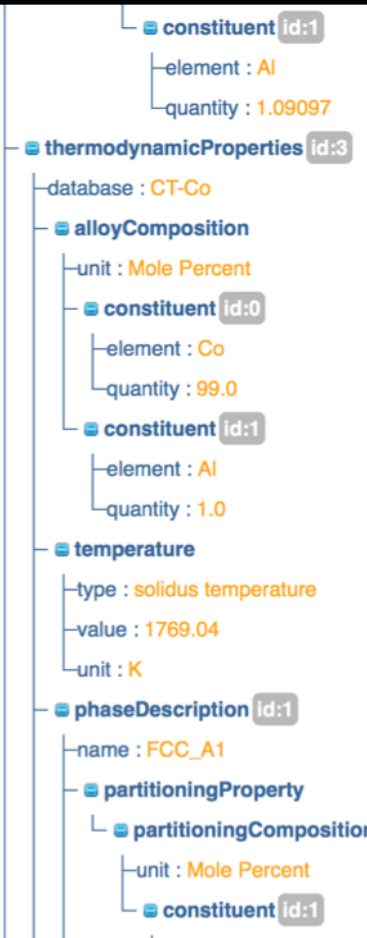
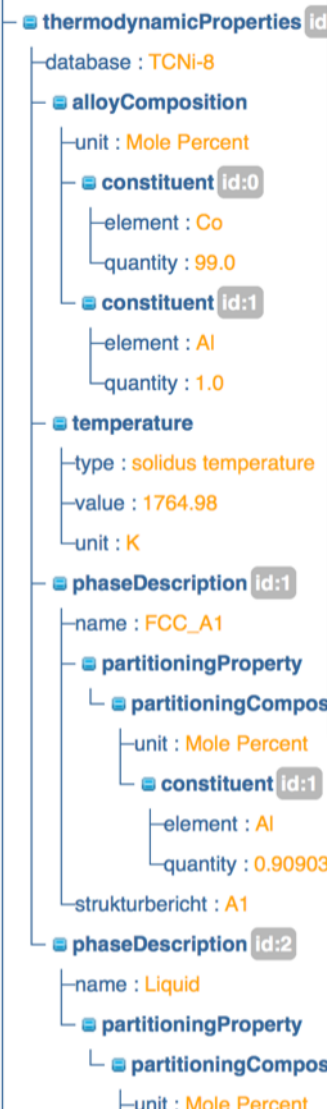
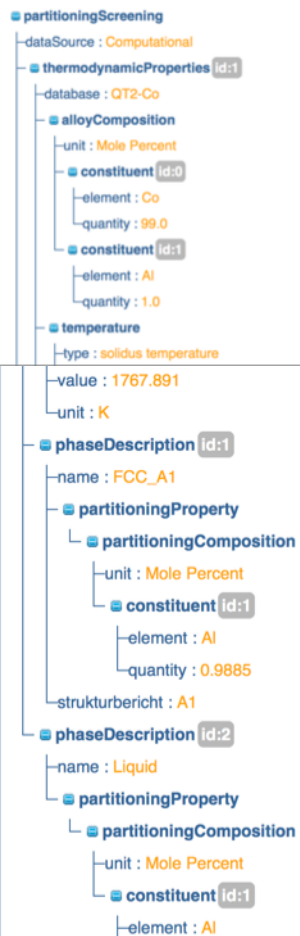
Data Representation for AI Liquid Partitioning Behavior

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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

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Home | **Data Curation** | Data Exploration | Composer

Select Template | **Enter Data** | View Data

Data Curation

- 1 Select Template
- 2 **Enter Data**
- 3 View Data

Data Entry

Here you can fill in the Materials Data form. Once it is completed, you can go to 'View Data' to review what you have entered. You won't be able to reach the review page before the document is valid according to the selected template. From the review page, you will be able to curate the data. The 'Save Form' button allows you to save partial data that you may want to edit later. This will only save a temporary document and won't actually curate data. All grayed elements are optional. Thus, all elements written in black are required. The document may still be valid with empty elements. There are no validation on empty fields if no such constraint is defined in the template. Thus, an empty string of characters may not raise a validation error, but an empty number will.

Clear Fields | Save Form | Download

- DiffusionCouple
 - SampleId
 - Id
 - SampleOwner
 - Date
 - Material
 - MaterialName
 - NominalComposition
 - Phase
 - AlloyForm
 - Material
 - MaterialName
 - NominalComposition
 - Phase
 - AlloyForm

Self Diffusion Resource

<http://www.ctcms.nist.gov/~gkl/selfdiffusion.html>

OVERVIEW SELF-DIFFUSION CONTACT

Self-Diffusion Data

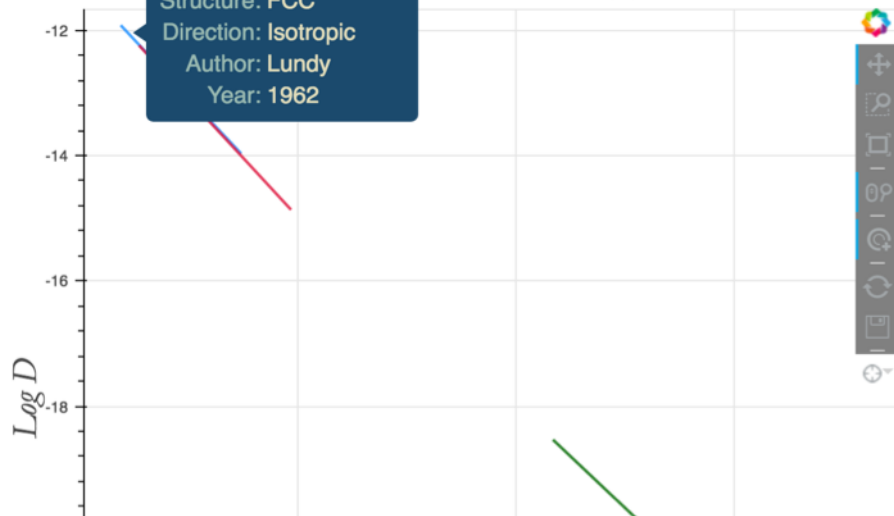
Method	Structure	Diffusion Direction	Frequency Factor D0 (m ² /s)	Activation Energy Q (kJ/mole)	Temperature (K)	Details	Reference	Raw data
--------	-----------	---------------------	---	-------------------------------	-----------------	---------	-----------	----------

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...	MDCS
Experime...	fcc	isotropic	2.200e-04	144.4	673 - 883	26Al. Dried-on from...	M. Beveler, Y. Adda...	MDCS
Experime...	fcc	isotropic	1.760e-05	126.5	358 - 482	Al. Void shrinkage (...)	T.E. Volin, R.W. Ball...	MDCS
Experime...	fcc	isotropic	1.370e-05	123.6	515 - 770	Al. NMR. SLRT (27A...	R. Messer et al.: Pr...	MDCS
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. Aqre...	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

Method: Experimental
 Structure: FCC
 Direction: Isotropic
 Author: Lundy
 Year: 1962

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

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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 isotopes necessitated use of a thick layer technique. The exact solution to in treating the data. Temperature dependence of the diffusion coefficients $-(34000/RT)DMn54=0.22exp-(28800/RT)$.
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

127.0.0.1

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

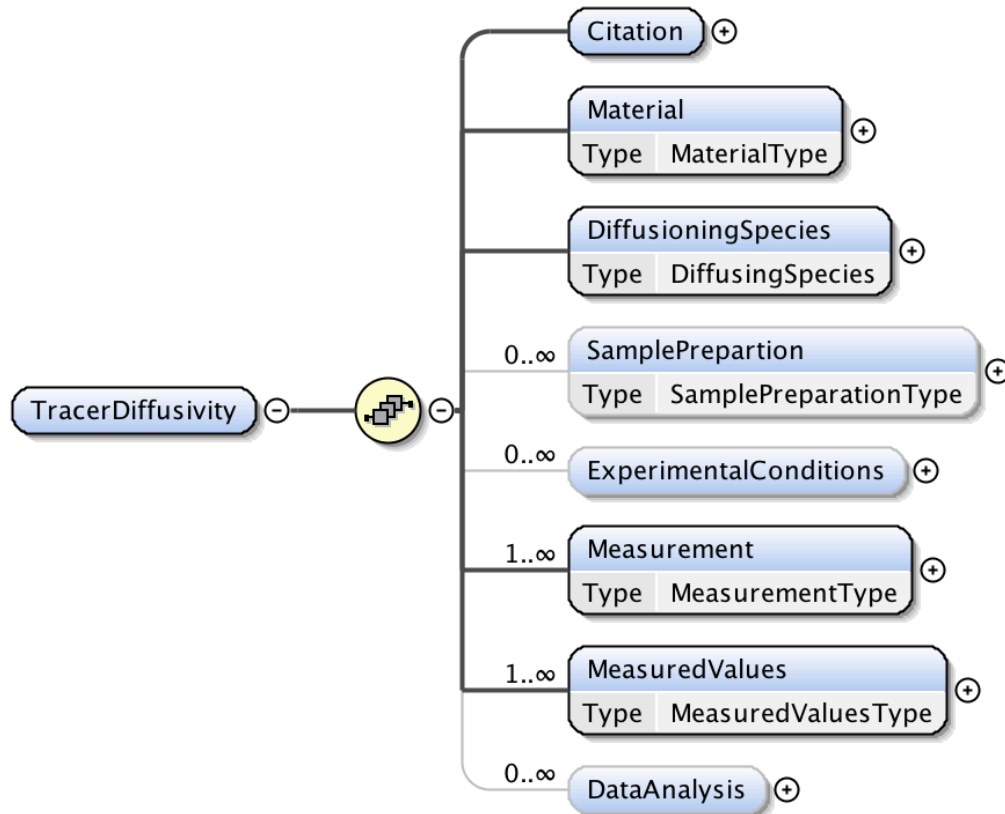
↓ Export

19 results (Select/Unselect all)

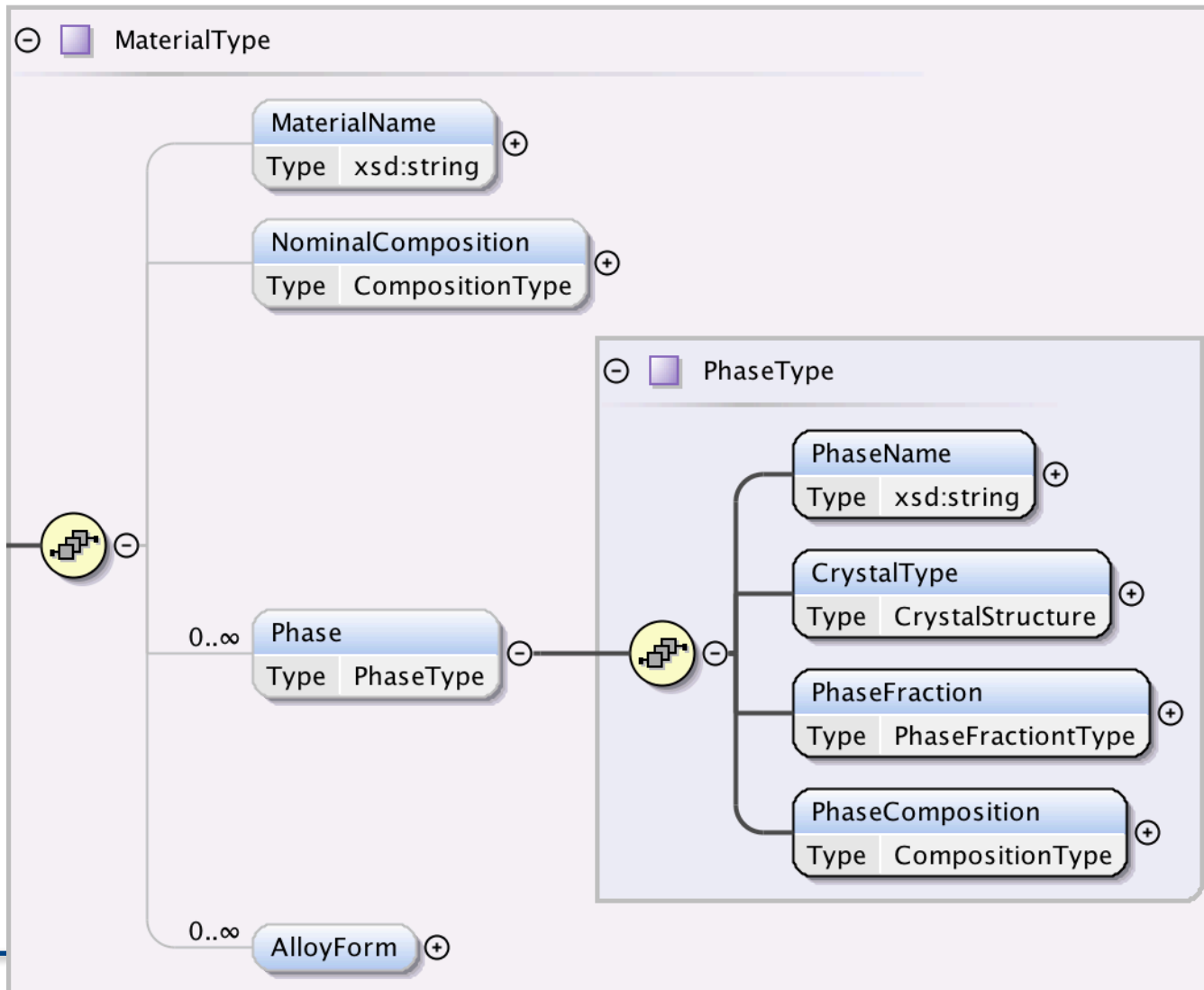
- [Ni-Bakker1968.xml](#) TracerImpurity-Lit
- [Ni-Monma-1964.xml](#) TracerImpurity-Lit
- [Ni-Hirano-1961.xml](#) TracerImpurity-Lit
- [Ni-Messener-1961.xml](#) TracerImpurity-Lit
- [Ni-MacEwan2-1959.xml](#) TracerImpurity-Lit
- [Ni-Hoffman-1956.xml](#) TracerImpurity-Lit
- [Ni-Reyonlds-1957.xml](#) 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
- [AlLundy1962.xml](#) TracerDiffusivityMod
- [AlBeyeler1968.xml](#) TracerDiffusivity2
- [Al-Messer-1974.xml](#) TracerDiffusivityMod
- [GE-DiffusionCouple-IN718-R95.xml](#) DiffusionDemo

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

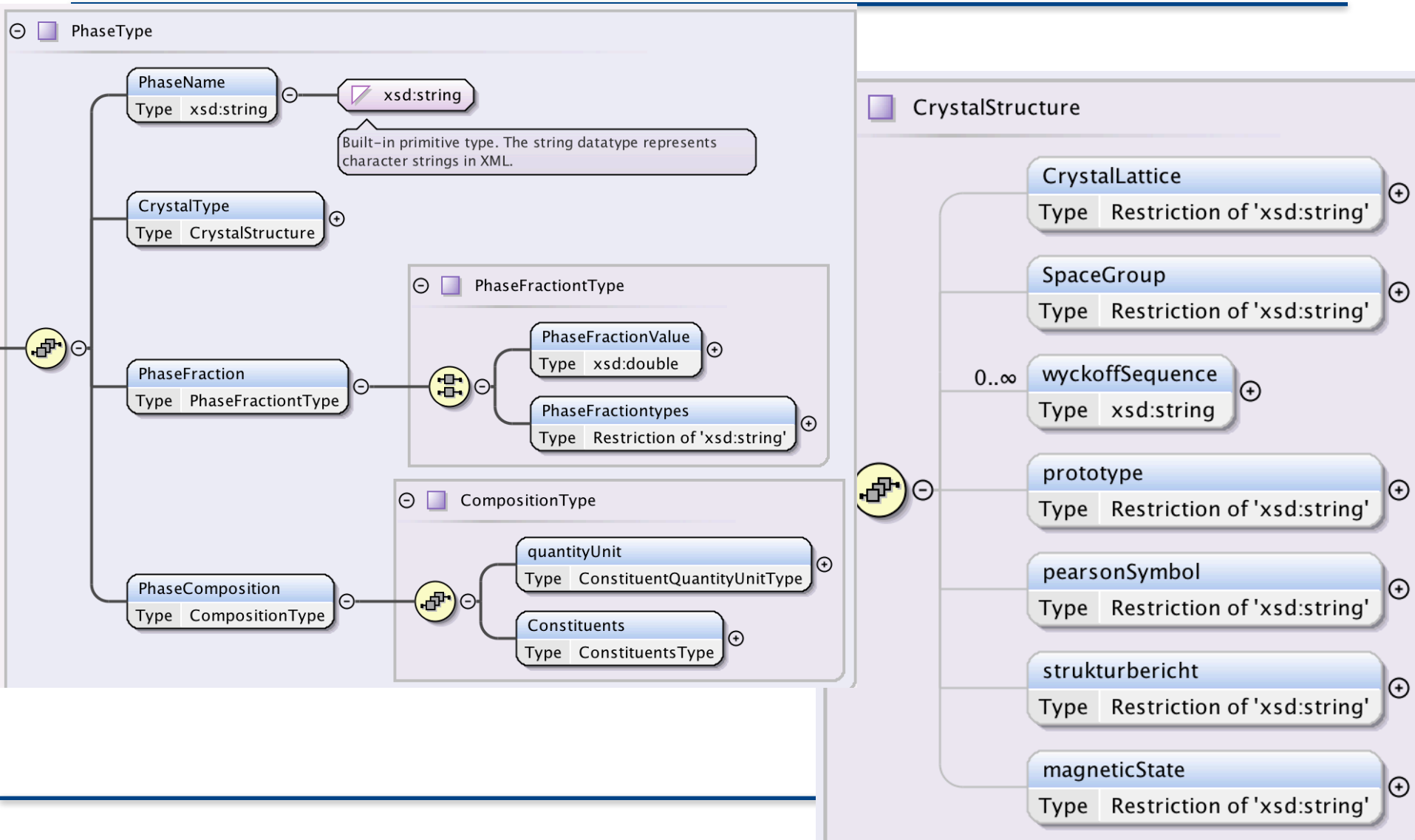
Tracer/Impurity Diffusion Literature



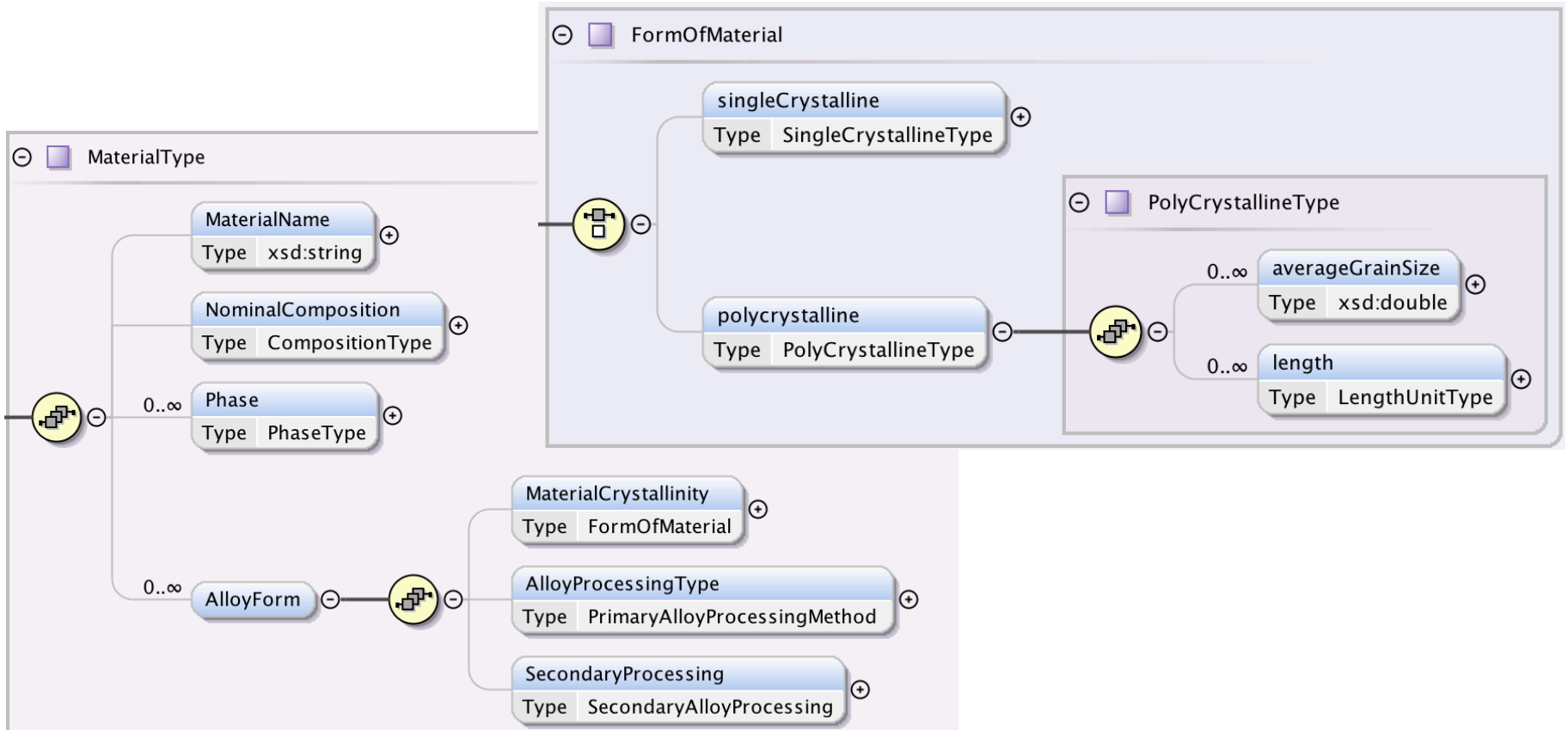
Material Description

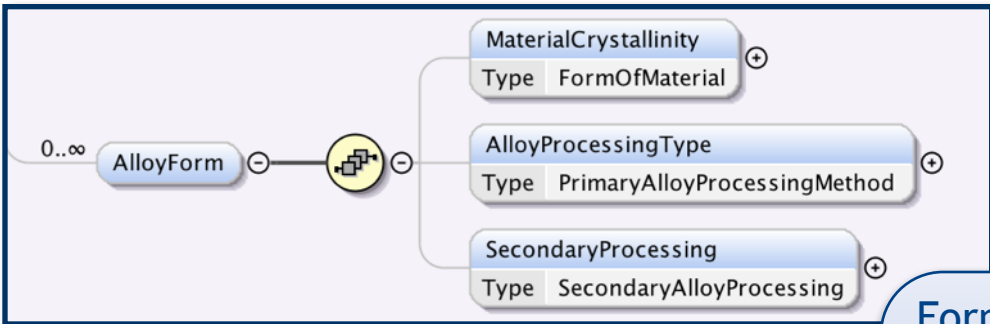


Material/Phase Type and Crystal Structure



Alloy Form

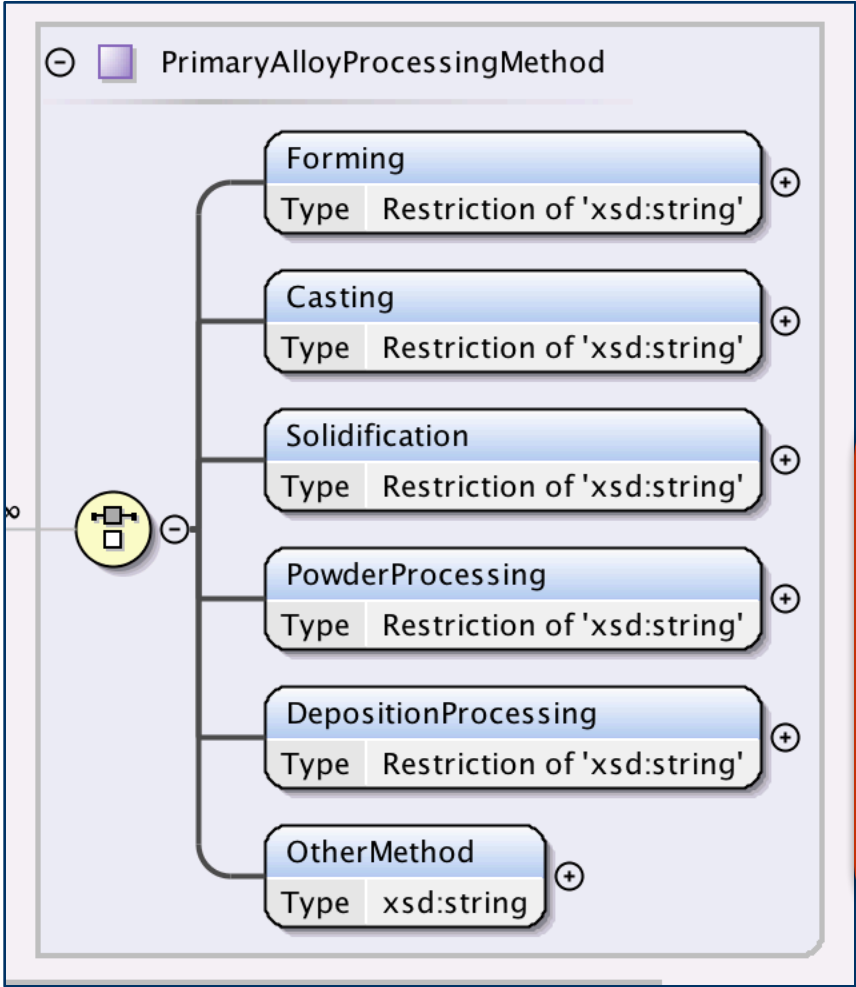




- ### Powder Processing
- Atomization
 - Ball Milling
 - Sponge Iron Process
 - Centrifugal Disintegration

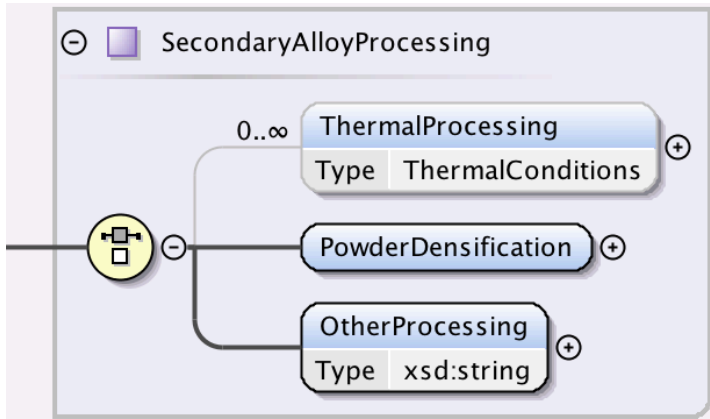
- ### Forming
- Forging
 - Cold Rolling
 - Hot Rolling
 - Extrusion
 - Drawing
 - Milling

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



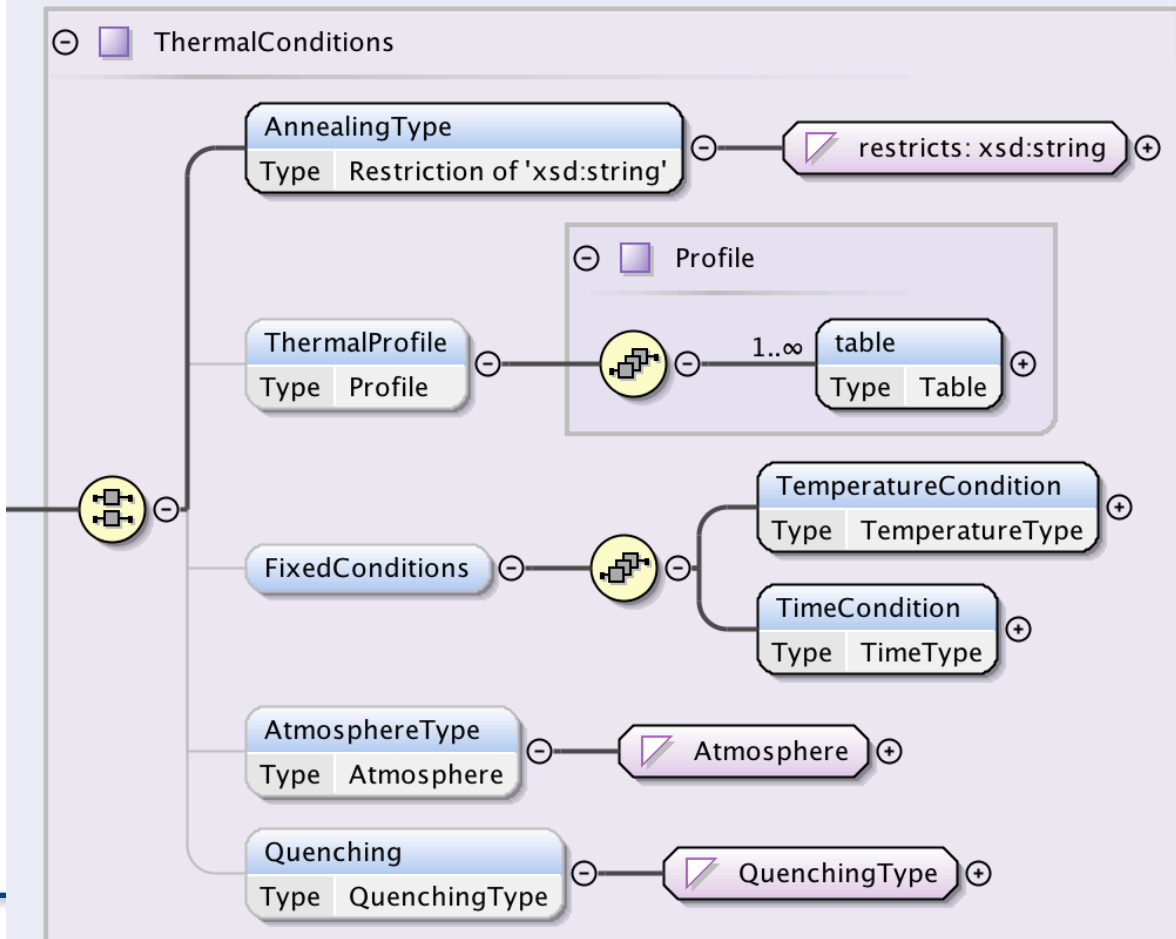
- ### Solidification
- Seeded Solidification
 - Directional Solidification
 - Zone Refining
 - Single Crystal Solidification
 - Rapid Solidification

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



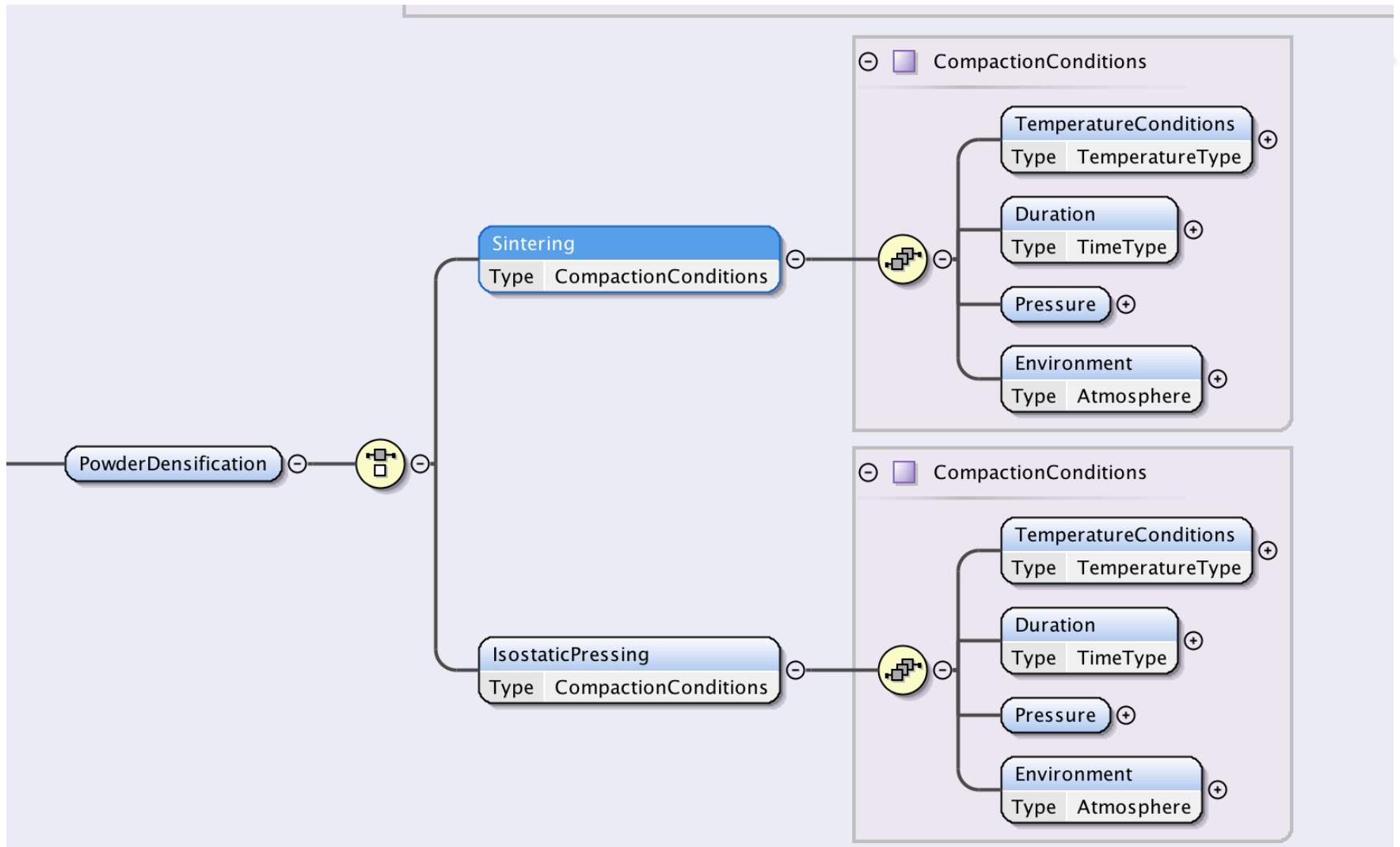
Annealing Type

- 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](#)