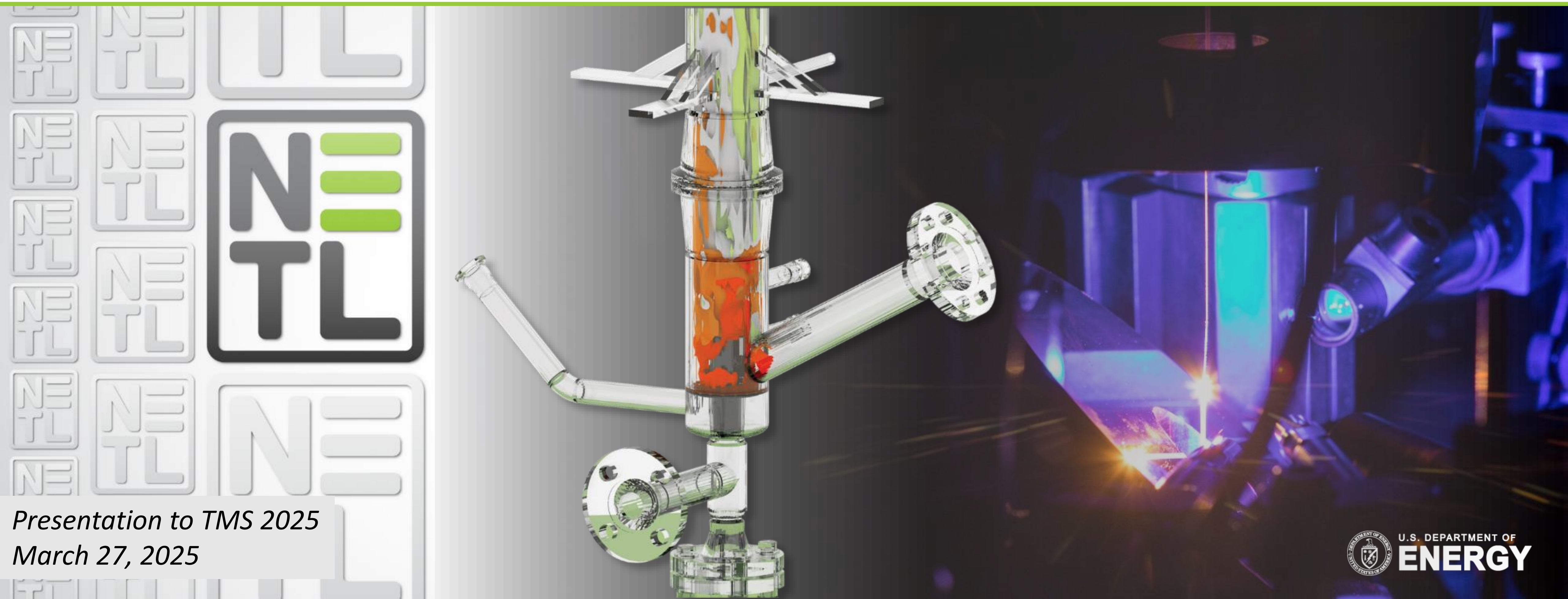
Developing an oxidation materials ontology for data-driven materials design

Madison Wenzlick
Research Engineer



Presentation to TMS 2025
March 27, 2025

Legal Disclaimer

Authors and Affiliations

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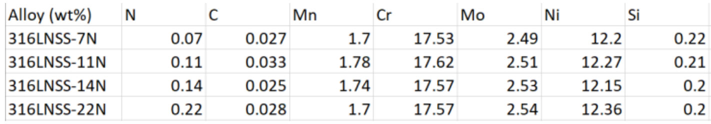
[3]NETL Support Contractor, 626 Cochran Mill Road, Pittsburgh, PA 15236

Materials Data Challenge



Alloy (wt%)	N	C	Mn	Cr	Mo	Ni	Si
316LNSS-7N	0.07	0.027	1.7	17.53	2.49	12.2	0.22
316LNSS-11N	0.11	0.033	1.78	17.62	2.51	12.27	0.21
316LNSS-14N	0.14	0.025	1.74	17.57	2.53	12.15	0.2
316LNSS-22N	0.22	0.028	1.7	17.57	2.54	12.36	0.2

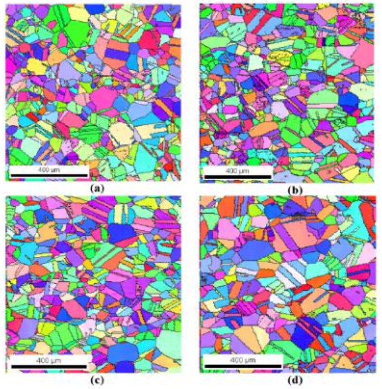
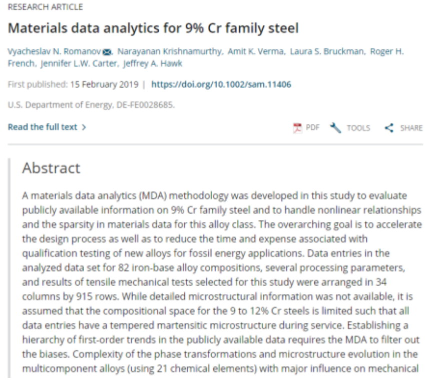


Fig. 1. Orientation imaging micrographs of solution annealed 316LN SS containing nitrogen (wt.%) of (a) 0.07, (b) 0.11, (c) 0.14 and (d) 0.22 N. Nearly equiaxed grains and annealing twins have been observed.



RESEARCH ARTICLE

Materials data analytics for 9% Cr family steel

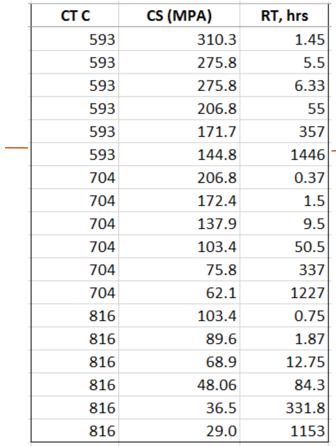
Vyacheslav N. Romanov, Narayanan Krishnamurthy, Amit K. Verma, Laura S. Bruckman, Roger H. French, Jennifer L.W. Carter, Jeffrey A. Hawk

First published: 15 February 2019 | https://doi.org/10.1002/sam.11406

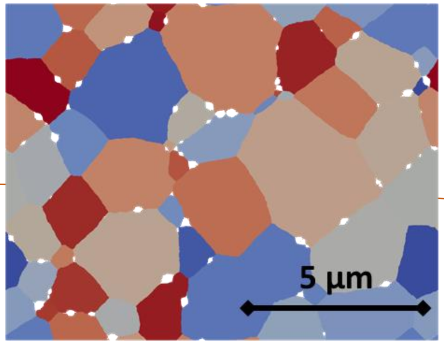
U.S. Department of Energy, DE-FE0028685.

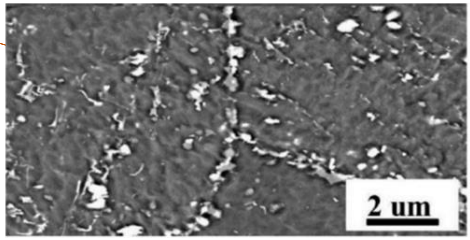
Abstract

A materials data analytics (MDA) methodology was developed in this study to evaluate publicly available information on 9% Cr family steel and to handle nonlinear relationships and the sparsity in materials data for this alloy class. The overarching goal is to accelerate the design process as well as to reduce the time and expense associated with qualification testing of new alloys for fossil energy applications. Data entries in the analyzed data set for 82 iron-base alloy compositions, several processing parameters, and results of tensile mechanical tests selected for this study were arranged in 34 columns by 915 rows. While detailed microstructural information was not available, it is assumed that the compositional space for the 9 to 12% Cr steels is limited such that all data entries have a tempered martensitic microstructure during service. Establishing a hierarchy of first-order trends in the publicly available data requires the MDA to filter out the biases. Complexity of the phase transformations and microstructure evolution in the multicomponent alloys (using 21 chemical elements) with major influence on mechanical

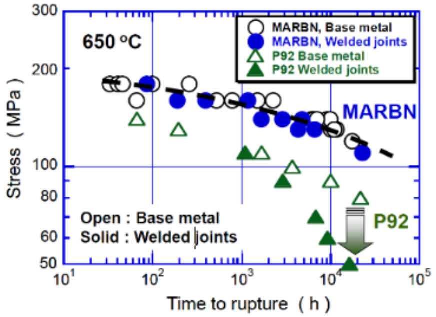


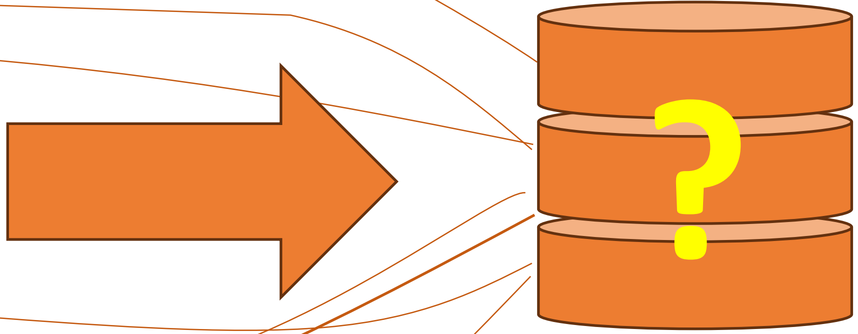
CT C	CS (MPA)	RT, hrs
593	310.3	1.45
593	275.8	5.5
593	275.8	6.33
593	206.8	55
593	171.7	357
593	144.8	1446
704	206.8	0.37
704	172.4	1.5
704	137.9	9.5
704	103.4	50.5
704	75.8	337
704	62.1	1227
816	103.4	0.75
816	89.6	1.87
816	68.9	12.75
816	48.06	84.3
816	36.5	331.8
816	29.0	1153





MARBN : 9Cr-3W-3Co-VNb, 120 - 150 ppm B & 60 - 90 ppm N
P92 : 9Cr-0.5Mo-1.8W-VNb, 20 ppm B & 500 ppm N





Materials Data Challenge Pt. 2

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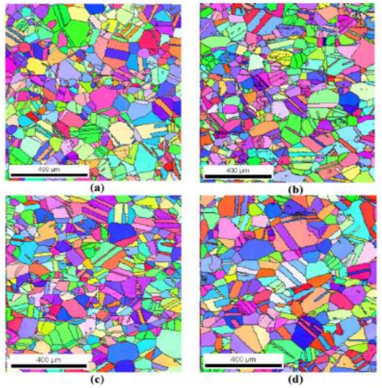

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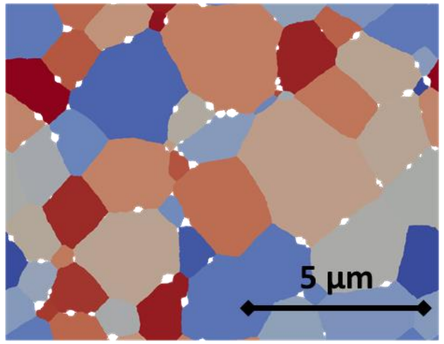
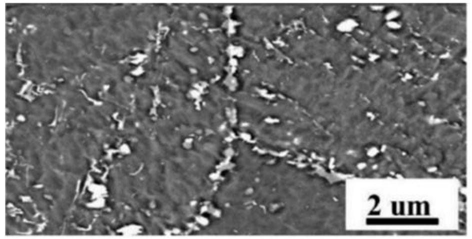
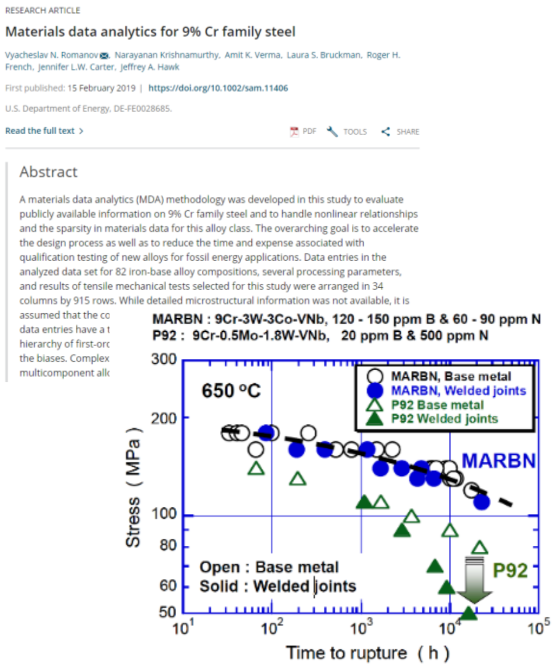




Project B



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Project C

Current challenge: data is siloed across projects; different researchers use different naming conventions; data is difficult to aggregate even within one group; metadata are scattered

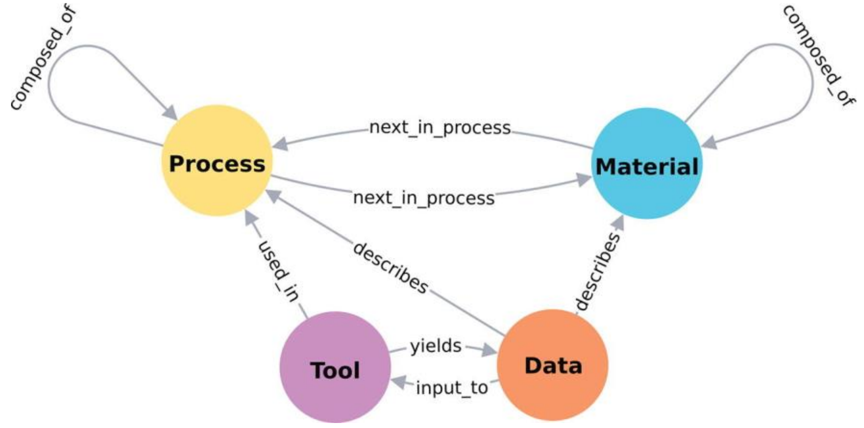
How to embed knowledge along with data?

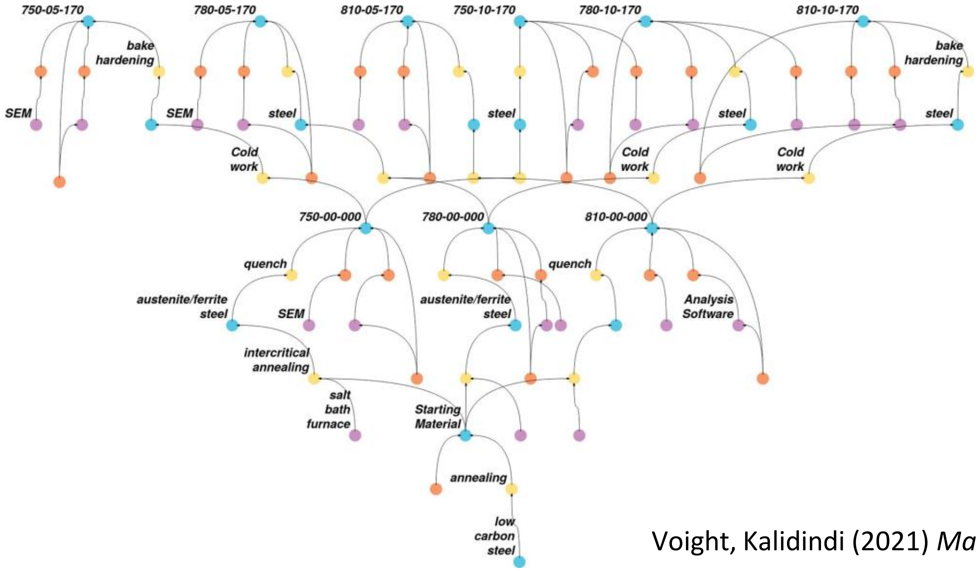
Ontology-Based Data Structure and Functions

Materials Ontology for Data Standardization

Supporting digitization & structure of collected data

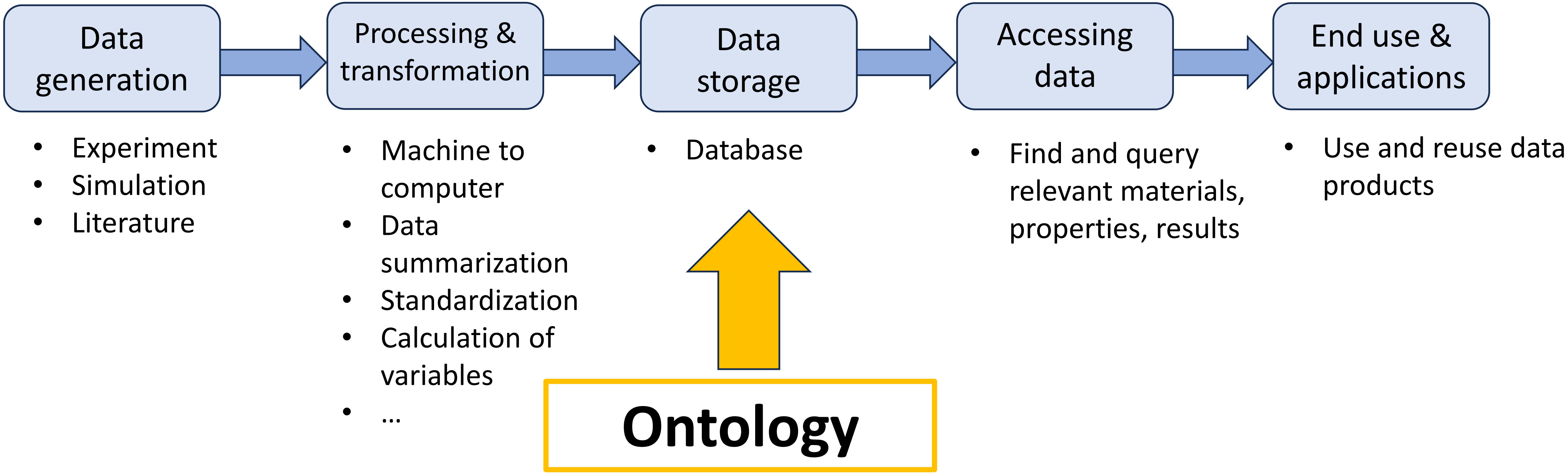
1. **Materials Ontology**
    - Standardization of naming convention for information
    - Indicate hierarchy and relationships of attributes
    - Capture metadata with data
    - Convey derivative information
    - Creating machine-interpretable digital data and human interpretable features
2. **Data Management Framework**
    - Apply graph-based data structure to relevant datasets
    - Explore digital connections between data generation, storage & use
    - Explore necessary data management techniques to optimize management of complex materials data





Voight, Kalidindi (2021) *Mat. Lett.*

Role of an ontology in a data workflow



Data generation

- Experiment
- Simulation
- Literature

Processing & transformation

- Machine to computer
- Data summarization
- Standardization
- Calculation of variables
- …

Data storage

- Database

Accessing data

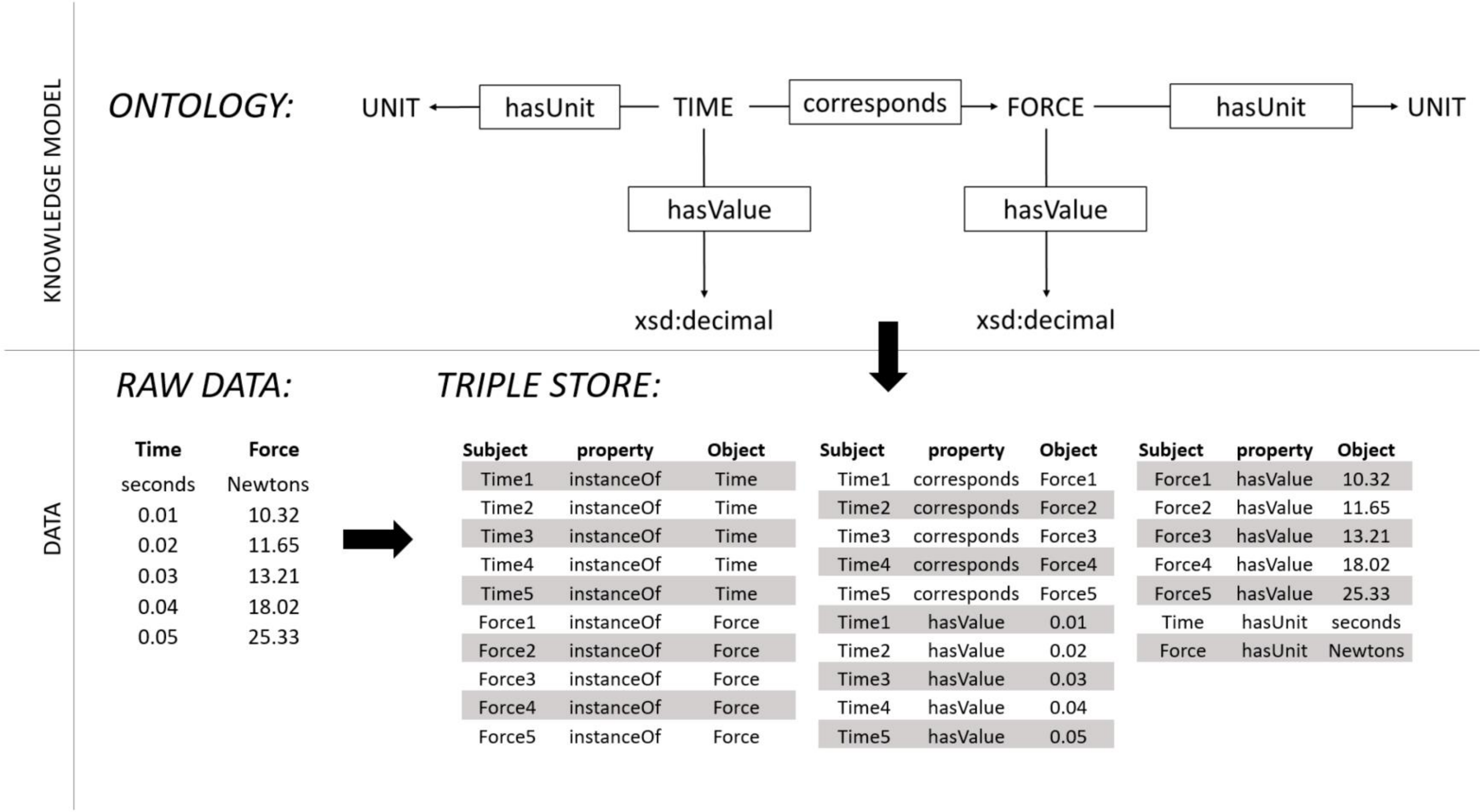
- Find and query relevant materials, properties, results

End use & applications

- Use and reuse data products

Ontology

How an Ontology Relates to Data

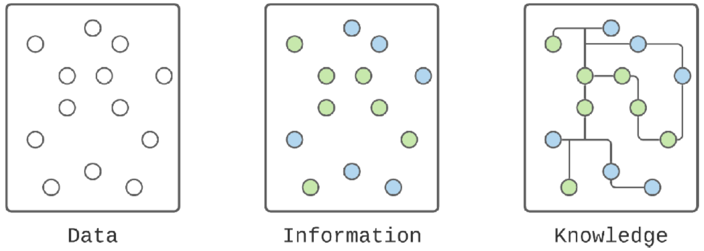


Time	Force
seconds	Newtons
0.01	10.32
0.02	11.65
0.03	13.21
0.04	18.02
0.05	25.33

Subject	property	Object
Time1	instanceOf	Time
Time2	instanceOf	Time
Time3	instanceOf	Time
Time4	instanceOf	Time
Time5	instanceOf	Time
Force1	instanceOf	Force
Force2	instanceOf	Force
Force3	instanceOf	Force
Force4	instanceOf	Force
Force5	instanceOf	Force

Subject	property	Object
Time1	corresponds	Force1
Time2	corresponds	Force2
Time3	corresponds	Force3
Time4	corresponds	Force4
Time5	corresponds	Force5
Time1	hasValue	0.01
Time2	hasValue	0.02
Time3	hasValue	0.03
Time4	hasValue	0.04
Time5	hasValue	0.05

Subject	property	Object
Force1	hasValue	10.32
Force2	hasValue	11.65
Force3	hasValue	13.21
Force4	hasValue	18.02
Force5	hasValue	25.33
Time	hasUnit	seconds
Force	hasUnit	Newtons



Voight, Kalidindi (2021) *Mat. Lett. c*

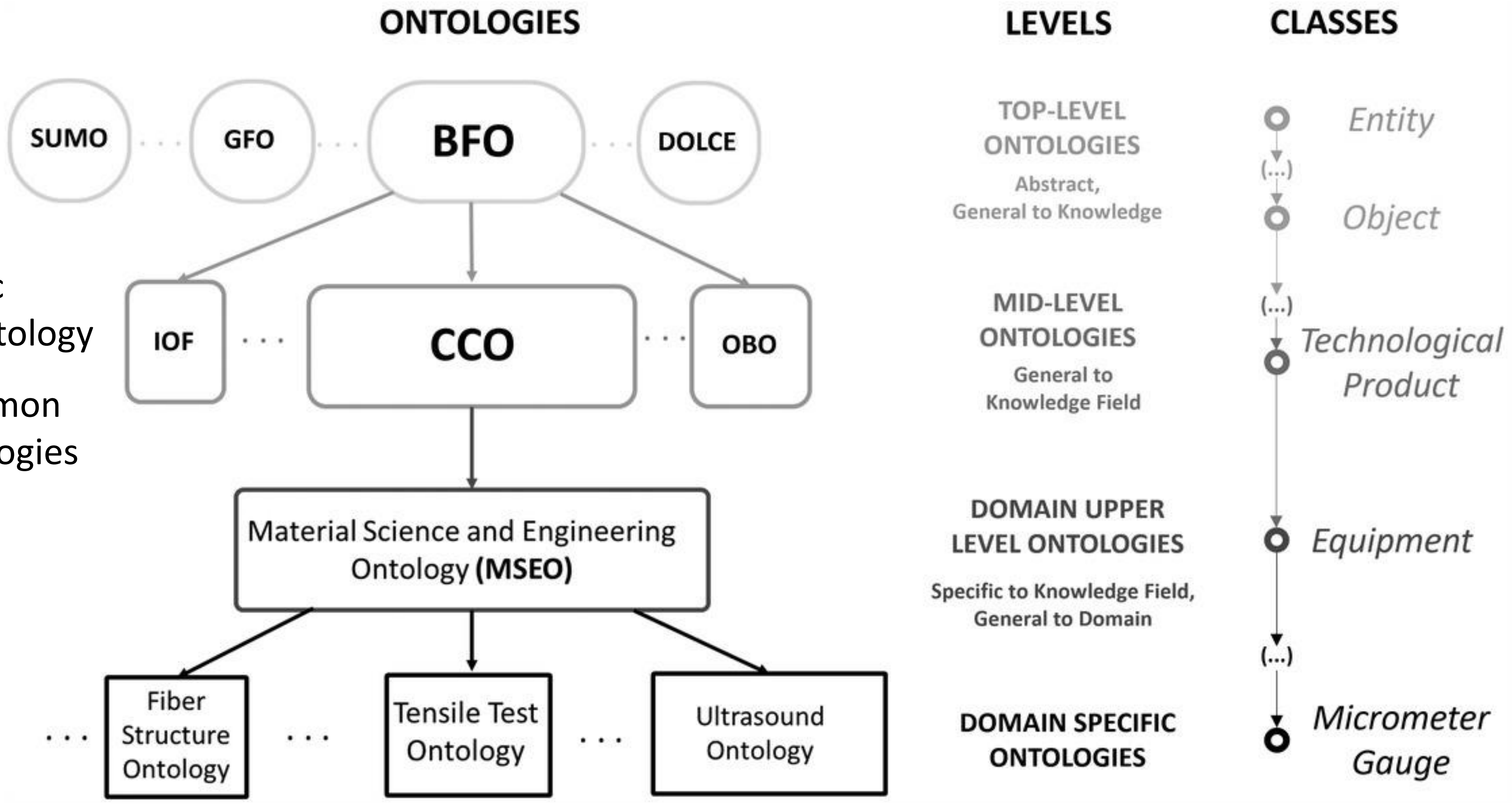
https://www.mdpi.com/2072-4292/13/12/2426

Integration with Established Ontologies

Beyerlein, B et al. 2022

BFO: basic formal ontology

CCO: common core ontologies



PROV O
Provenance Ontology

↓

PMD-Co
Platform MaterialDigital Core Ontology

↓

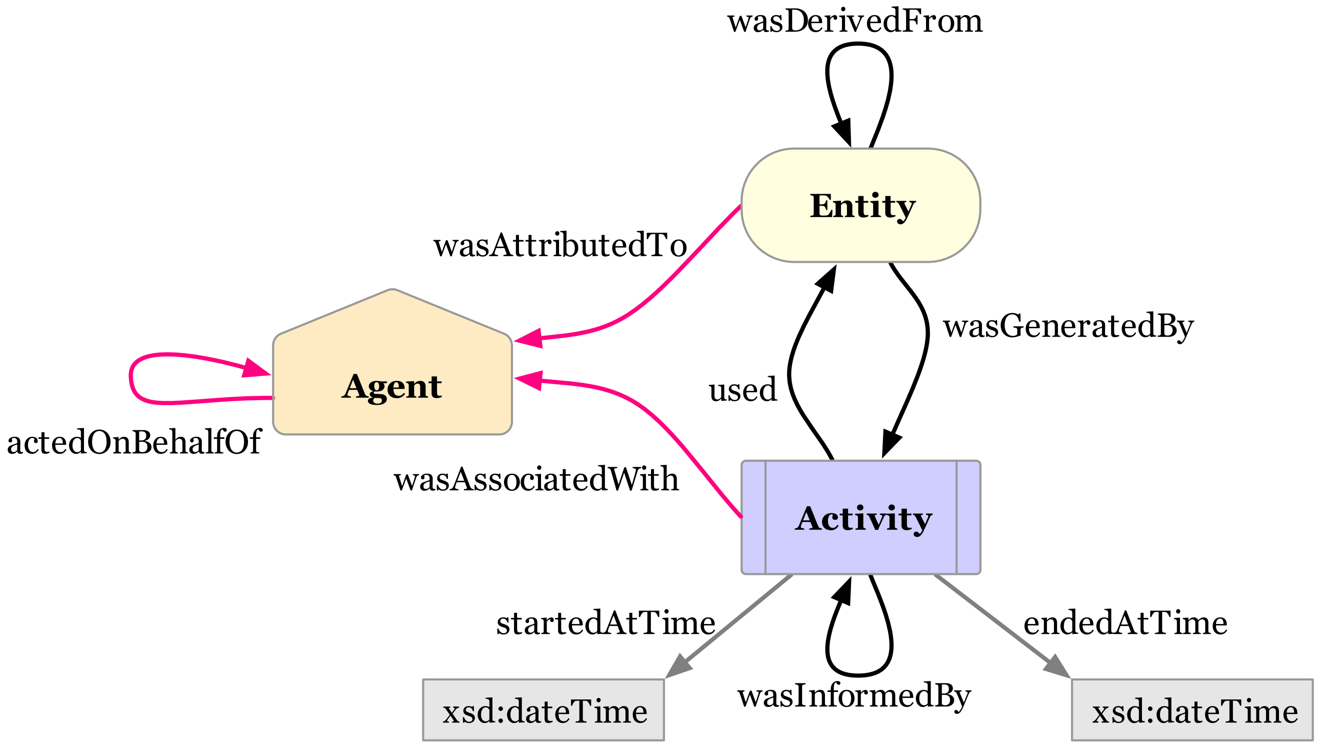
Materials Oxidation Ontology

Beyerlein, B et a. 2022 https://onlinelibrary.wiley.com/doi/full/10.1002/adem.202101176

PROV-O Logic Structure

Provenance Ontology

- Agent – Activity – Entity
- Procedure focused
- Easily capture complex processing steps, testing steps

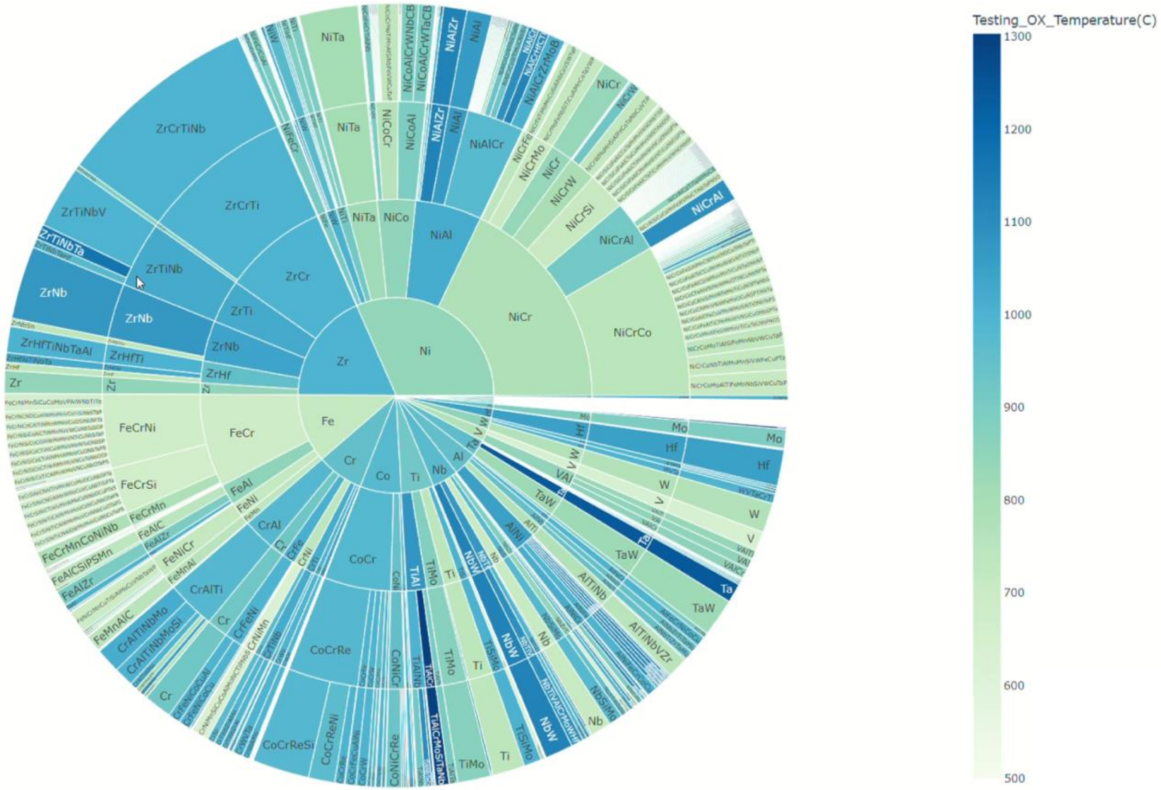


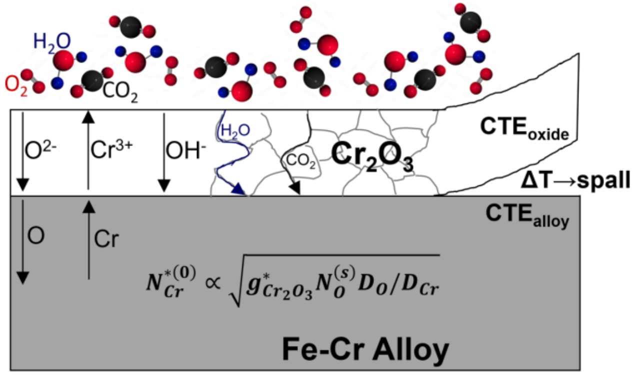
https://www.w3.org/TR/prov-o/

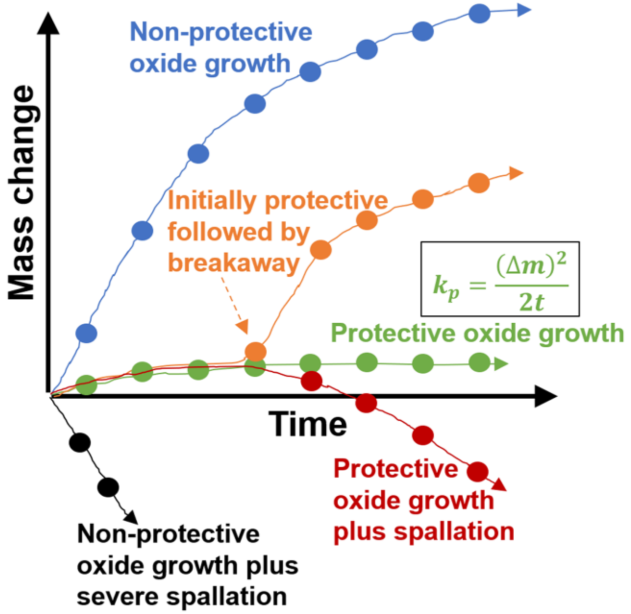
Data Collected: Alloy Oxidation

- ~40,000 data points
  - 7,000 from NETL in-house testing
  - 33,000 from literature

- Variety of testing environments: air, Ar, CO_2
- Responses include mass gain and k_p







Oxidation Database Details: Example Attributes

Composition

- Element nickel (Ni)
- Element chromium (Cr)
- Element cobalt (Co)
- Element molybdenum (Mo)
- Element titanium (Ti)
- Element aluminum (Al)
- Element iron (Fe)
- Element manganese (Mn)
- Element silicon (Si)
- Element carbon (C)
- Element boron (B)
- Element phosphorous (P)
- Element copper (Cu)
- Element tungsten (W)
- Element nitrogen (N)
- Element niobium (Nb)
- Element vanadium (V)
- Element sulfur (S)
- Element yttrium (Y)
- Element zirconium (Zr)
- …
- Element tantalum (Ta)
- Element lanthanum (La)
- Element platinum (Pt)
- Element rhenium (Re)
- Element tin (Sn)

Composition - Oxides

- Oxide TiO2
- Oxide Cr2O3
- Oxide Al2O3
- Oxide Gd2O3
- Oxide La2O3
- Oxide ZrO2
- Oxide SiO2
- Oxide Ta2O5
- Oxide Eu2O3
- Oxide Yb2O3
- Oxide Dy2O3
- Oxide Lu2O3
- Oxide Er2O3
- Oxide Ho2O3
- Oxide Tb2O3
- Oxide CeO2
- Oxide Sm2O3
- Oxide Y2O3
- Oxide MgO

Test Conditions & Environment

- Temperature (°C)
- 1000/T(K)
- Atmosphere name
- Pressure (atm)
- O2 (%)
- N2 (%)
- H2O (%)
- H2 (%)
- CO2 (%)
- CO (%)
- Ar (%)
- SO2 (%)
- Total exposure time (h)
- Number of thermal cycles

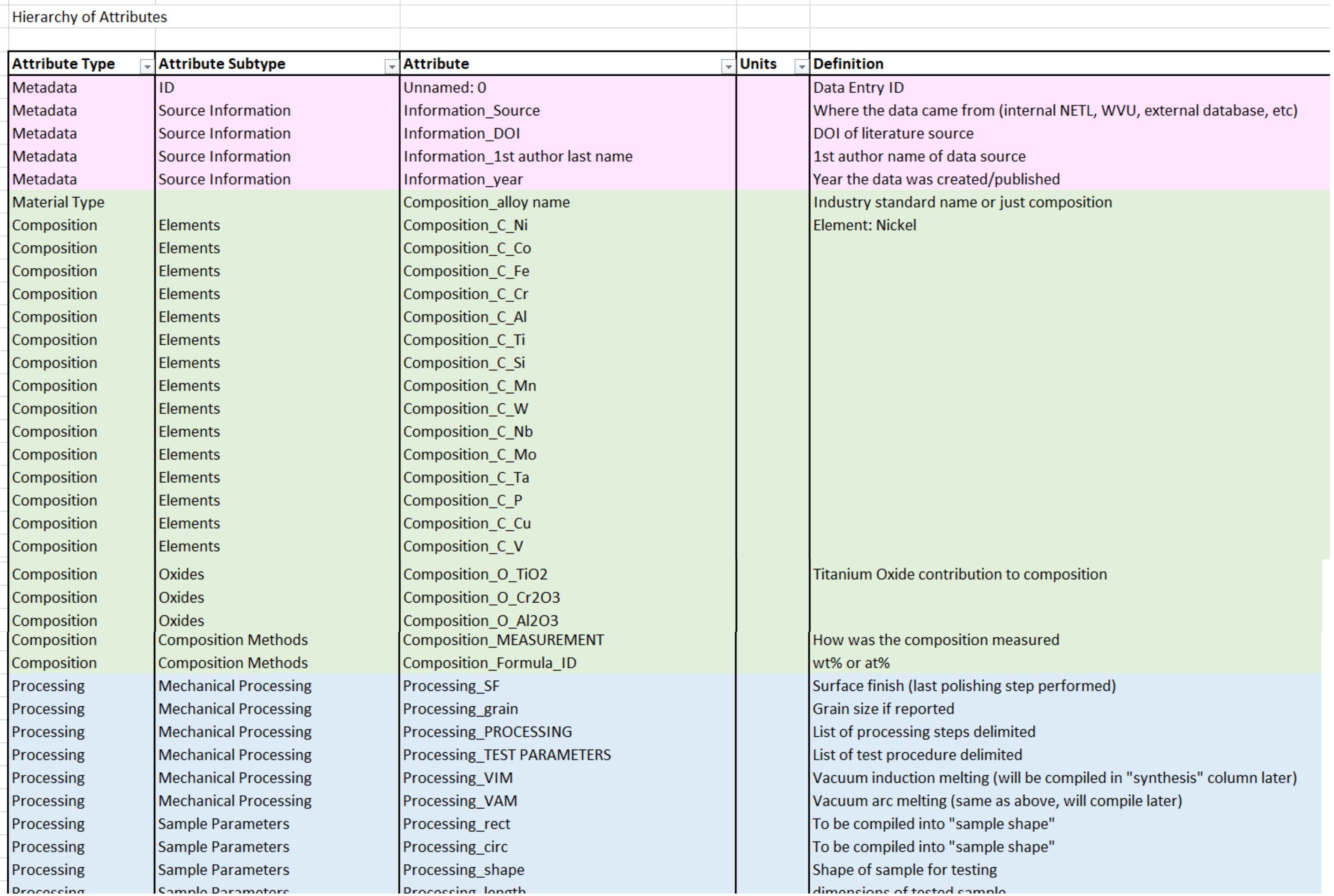
Alloy Information

- Surface finish (last polishing step performed)
- Grain size if reported
- List of processing steps delimited
- List of test procedure delimited
- Vacuum induction melting
- Vacuum arc melting
- Shape of sample for testing

Test Attributes

- Disintegration of sample time (refractories)
- Thickness of oxide
- Time before protective oxide layer formed
- Types of oxides formed
- Phases in alloy
- Mass change at end of exposure (mg/cm2)
- Parabolic check (Y/N)
- kp unit
- kp
- kp (g2/cm4/s)
- kp reported or calculated?
- R2 if kp calculated
- Comments

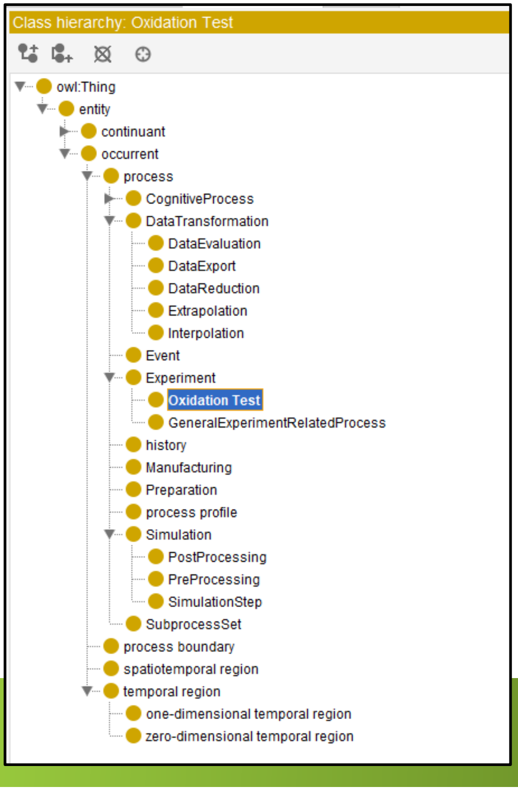
First steps



Hierarchy of Attributes

Attribute Type	Attribute Subtype	Attribute	Units	Definition
Metadata	ID	Unnamed: 0		Data Entry ID
Metadata	Source Information	Information_Source		Where the data came from (internal NETL, WVU, external database, etc)
Metadata	Source Information	Information_DOI		DOI of literature source
Metadata	Source Information	Information_1st author last name		1st author name of data source
Metadata	Source Information	Information_year		Year the data was created/published
Material Type		Composition_alloy name		Industry standard name or just composition
Composition	Elements	Composition_C_Ni		Element: Nickel
Composition	Elements	Composition_C_Co		
Composition	Elements	Composition_C_Fe		
Composition	Elements	Composition_C_Cr		
Composition	Elements	Composition_C_Al		
Composition	Elements	Composition_C_Ti		
Composition	Elements	Composition_C_Si		
Composition	Elements	Composition_C_Mn		
Composition	Elements	Composition_C_W		
Composition	Elements	Composition_C_Nb		
Composition	Elements	Composition_C_Mo		
Composition	Elements	Composition_C_Ta		
Composition	Elements	Composition_C_P		
Composition	Elements	Composition_C_Cu		
Composition	Elements	Composition_C_V		
Composition	Oxides	Composition_O_TiO2		Titanium Oxide contribution to composition
Composition	Oxides	Composition_O_Cr2O3		
Composition	Oxides	Composition_O_Al2O3		
Composition	Composition Methods	Composition_MEASUREMENT		How was the composition measured
Composition	Composition Methods	Composition_Formula_ID		wt% or at%
Processing	Mechanical Processing	Processing_SF		Surface finish (last polishing step performed)
Processing	Mechanical Processing	Processing_grain		Grain size if reported
Processing	Mechanical Processing	Processing_PROCESSING		List of processing steps delimited
Processing	Mechanical Processing	Processing_TEST PARAMETERS		List of test procedure delimited
Processing	Mechanical Processing	Processing_VIM		Vacuum induction melting (will be compiled in "synthesis" column later)
Processing	Mechanical Processing	Processing_VAM		Vacuum arc melting (same as above, will compile later)
Processing	Sample Parameters	Processing_rect		To be compiled into "sample shape"
Processing	Sample Parameters	Processing_circ		To be compiled into "sample shape"
Processing	Sample Parameters	Processing_shape		Shape of sample for testing
Processing	Sample Parameters	Processing_length		dimensions of tested sample

- Create legend for Oxidation data, including attribute names, units, and definitions
- Assign to types and subtypes as a part of the attribute hierarchy in the ontology



Class hierarchy: Oxidation Test

- owl:Thing
  - entity
    - continuant
    - occurrent
      - process
        - CognitiveProcess
        - DataTransformation
          - DataEvaluation
          - DataExport
          - DataReduction
          - Extrapolation
          - Interpolation
        - Event
        - Experiment
          - Oxidation Test
          - GeneralExperimentRelatedProcess
        - history
        - Manufacturing
        - Preparation
        - process profile
        - Simulation
          - PostProcessing
          - PreProcessing
          - SimulationStep
        - SubprocessSet
      - process boundary
      - spatiotemporal region
      - temporal region
        - one-dimensional temporal region
        - zero-dimensional temporal region

Ontology Structure

Framework of logic for defining information

Classes

- Activity
  - Process
    - Measuring process
- Agent
  - Organization
  - Data Source
- Entity
  - Object
  - Value Object
    - Atmosphere
    - Cooling Method
    - Cycle Number
    - Mass Change
    - …

Object Properties

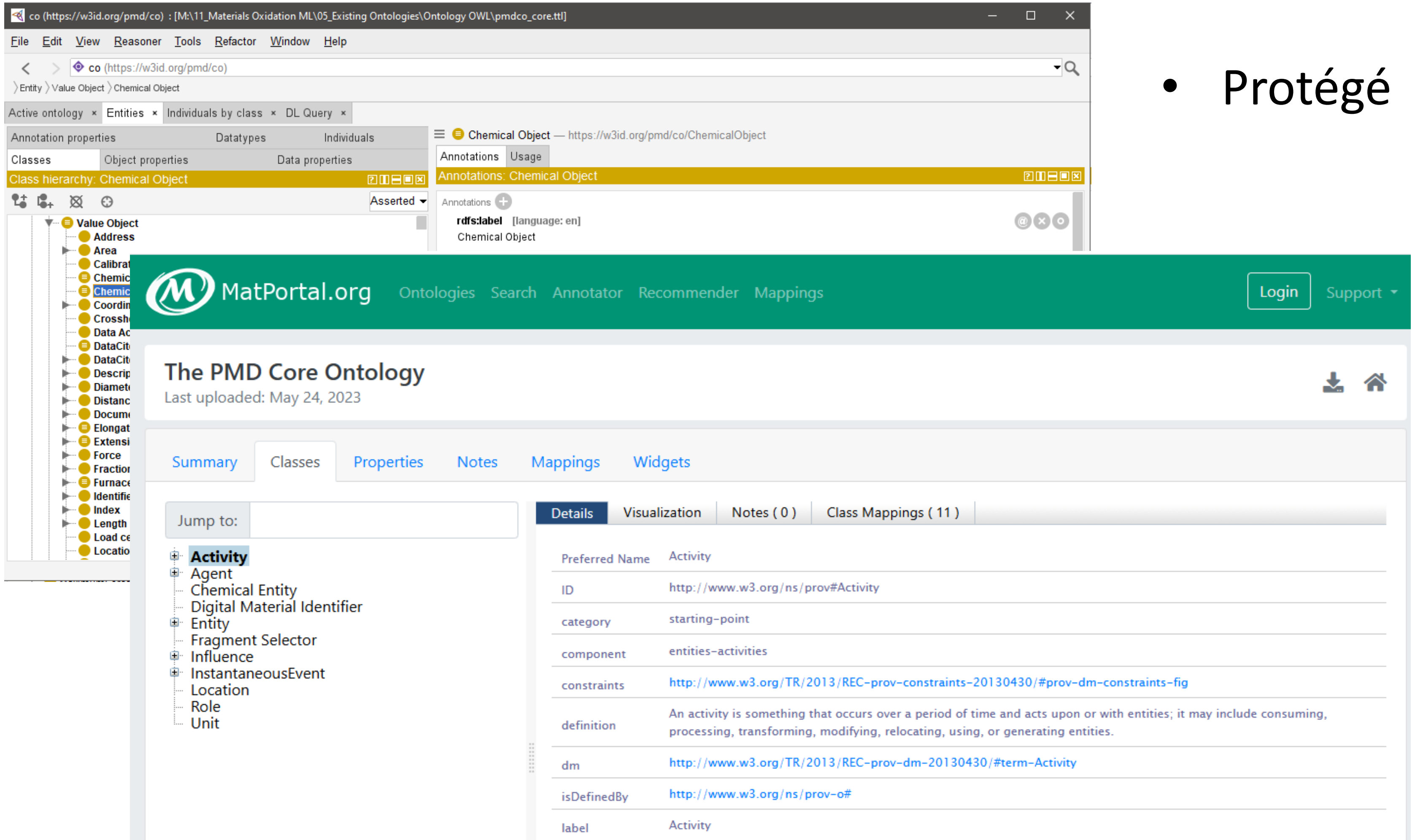
- hasSampleMaterial
  - hasAlloyName
- hasIdentifier
- Participant of
  - Input of
  - Output of
- Process
- Previous Process
- Next Process
- …

Data Properties

- Data quality
- Composition values
- Testing results

- **Experiment** is basis of data structure
- Many logical decisions needed when creating the ontology
- Importance of **domain knowledge** in ontology

Ontology Creation Tools



rdfs:label [language: en]
Chemical Object

- Value Object
  - Address
  - Area
  - Calibrat
  - Chemic
  - Chemic
  - Coordin
  - Crossh
  - Data Ac
  - DataCit
  - DataCit
  - Descrip
  - Diamet
  - Distanc
  - Docum
  - Elongat
  - Extensi
  - Force
  - Fraction
  - Furnace
  - Identifie
  - Index
  - Length
  - Load ce
  - Locatio

The PMD Core Ontology

Last uploaded: May 24, 2023

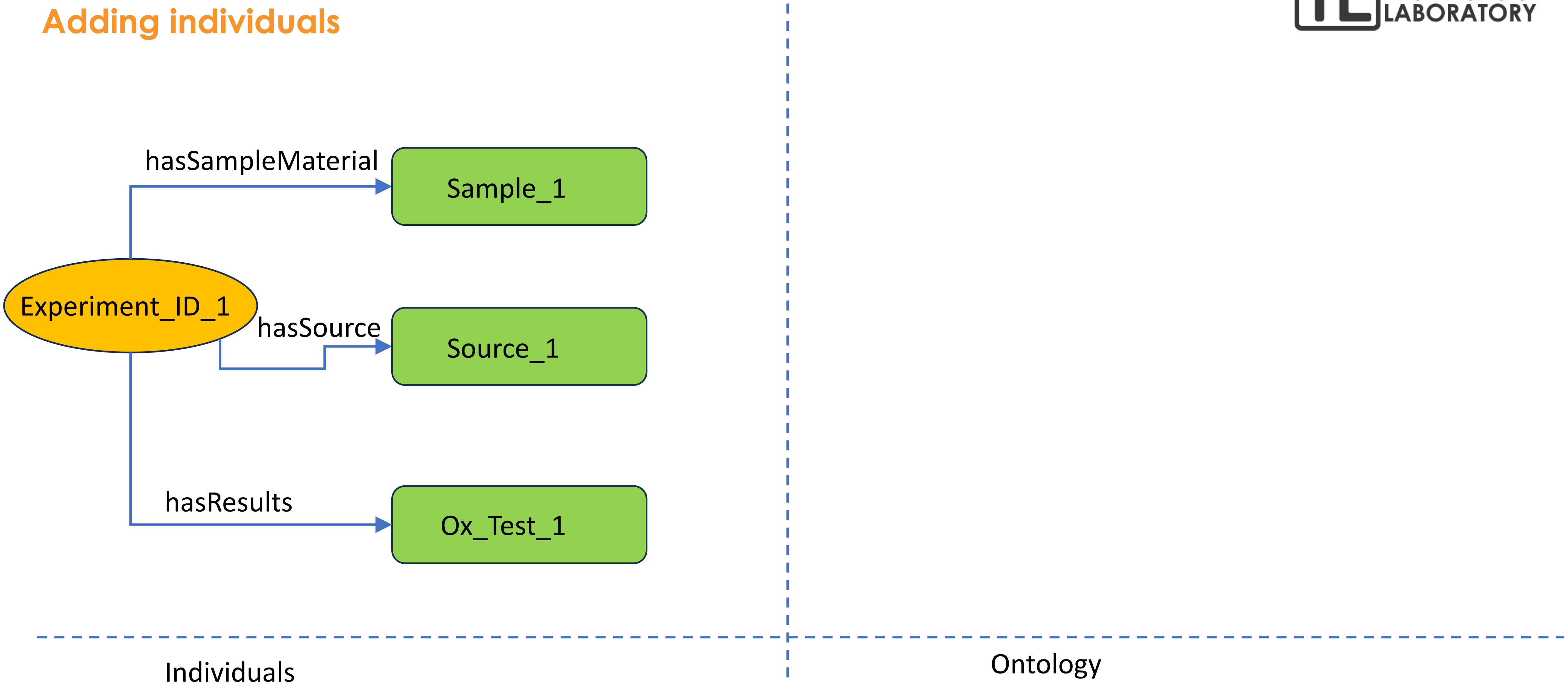
- Activity
- Agent
- Chemical Entity
- Digital Material Identifier
- Entity
- Fragment Selector
- Influence
- InstantaneousEvent
- Location
- Role
- Unit

Preferred Name	Activity
ID	http://www.w3.org/ns/prov#Activity
category	starting-point
component	entities-activities
constraints	http://www.w3.org/TR/2013/REC-prov-constraints-20130430/#prov-dm-constraints-fig
definition	An activity is something that occurs over a period of time and acts upon or with entities; it may include consuming, processing, transforming, modifying, relocating, using, or generating entities.
dm	http://www.w3.org/TR/2013/REC-prov-dm-20130430/#term-Activity
isDefinedBy	http://www.w3.org/ns/prov-o#
label	Activity

- Protégé
- MatPortal.org
- Python libraries
  - RDFlib
  - Owlready2

Representing Testing Data in the Ontology

Adding individuals



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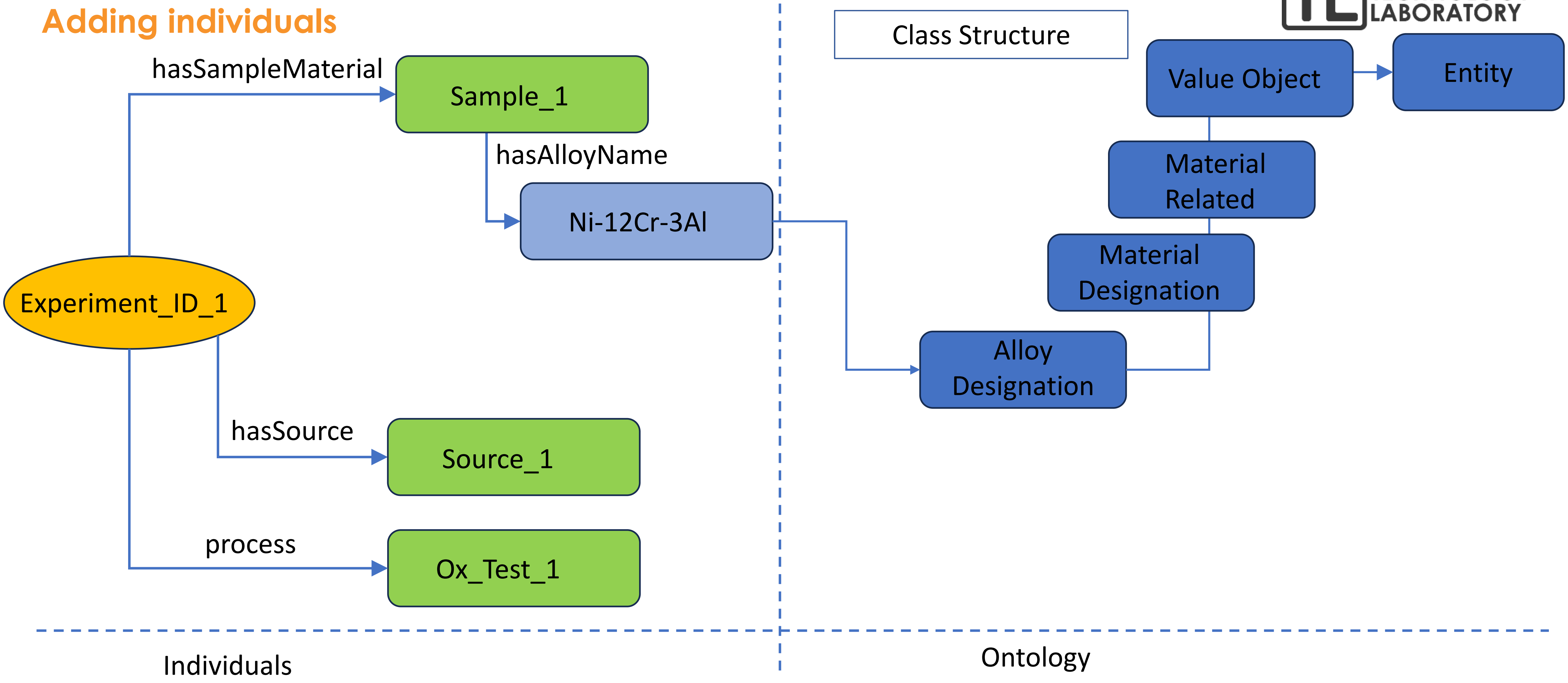

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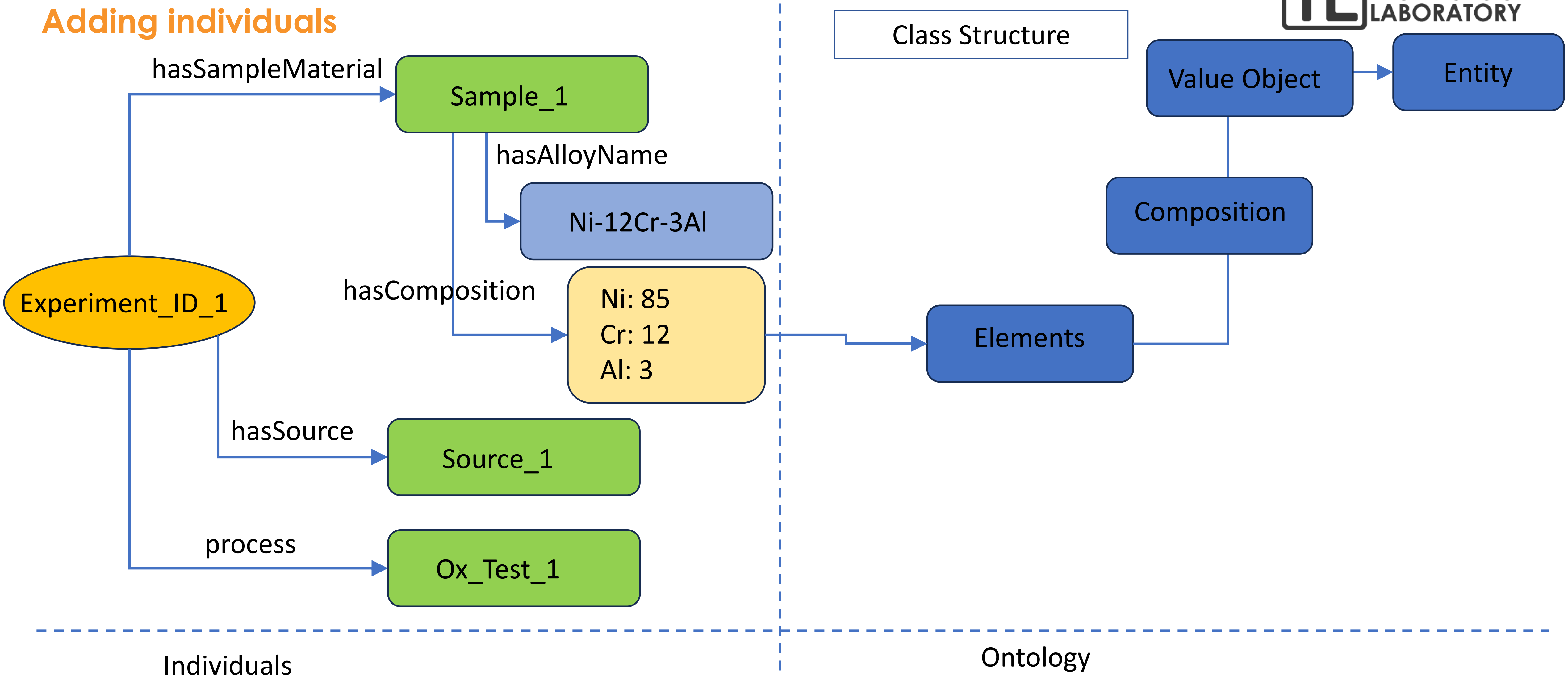


hasSampleMaterial

Sample_1

hasAlloyName

Ni-12Cr-3Al

Experiment_ID_1

hasComposition

Ni: 85
Cr: 12
Al: 3

hasSource

Source_1

process

Ox_Test_1

Class Structure

Value Object

Entity

Composition

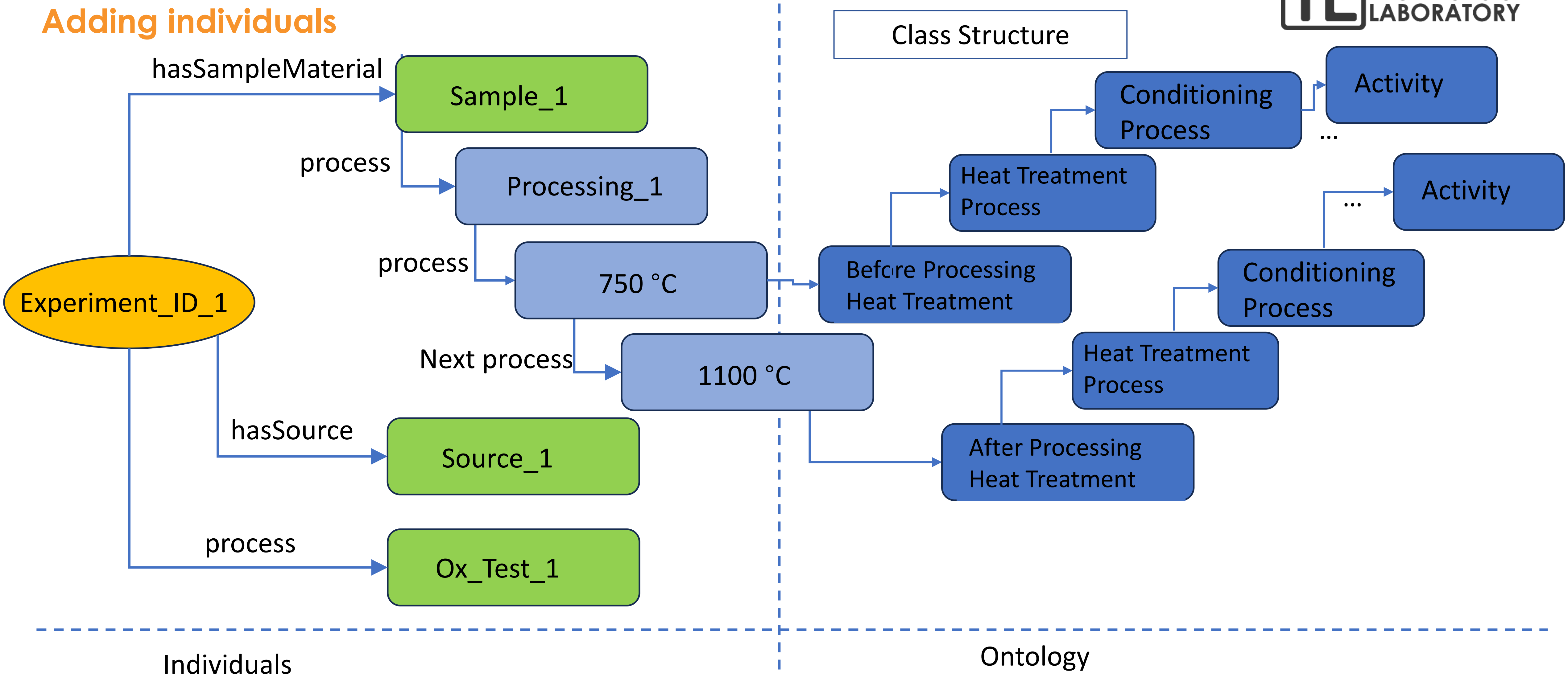
Elements

Individuals

Ontology

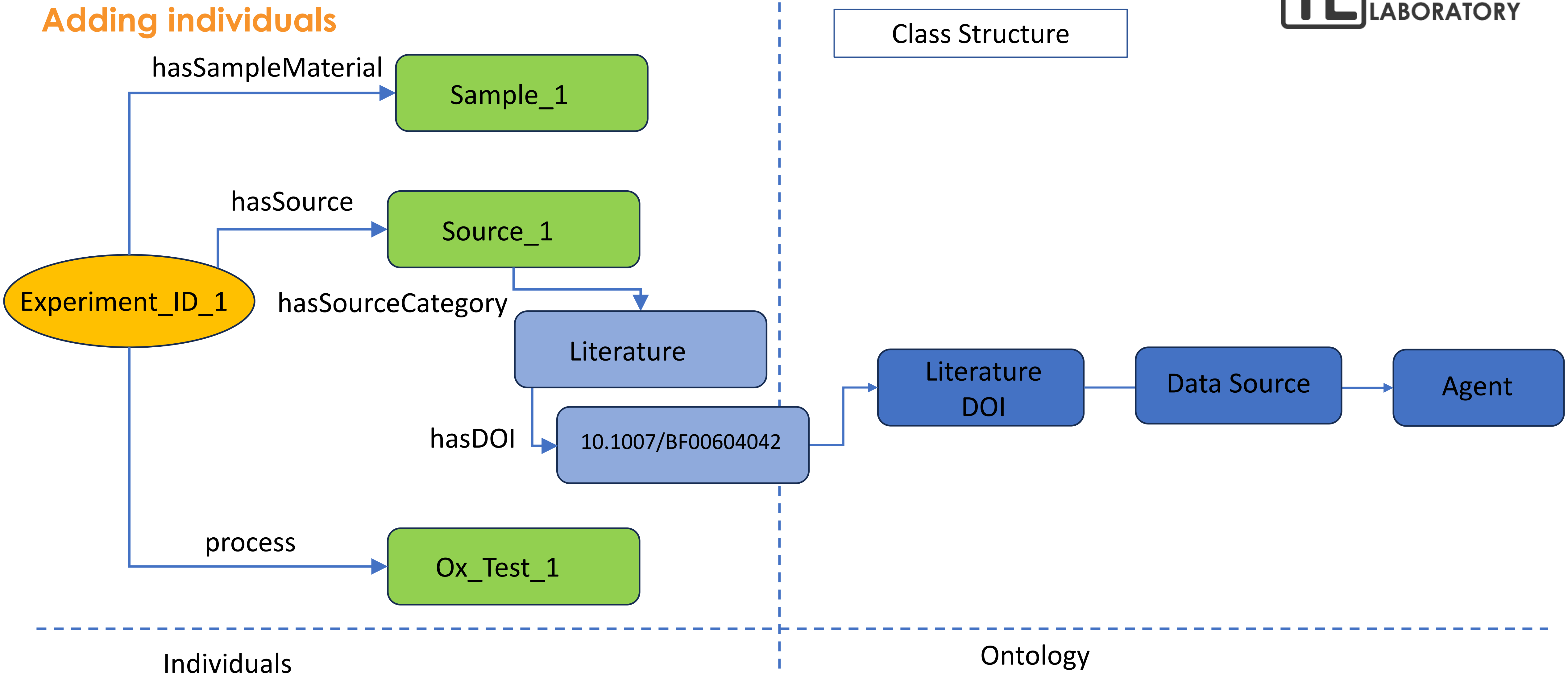
Representing Testing Data in the Ontology

Adding individuals



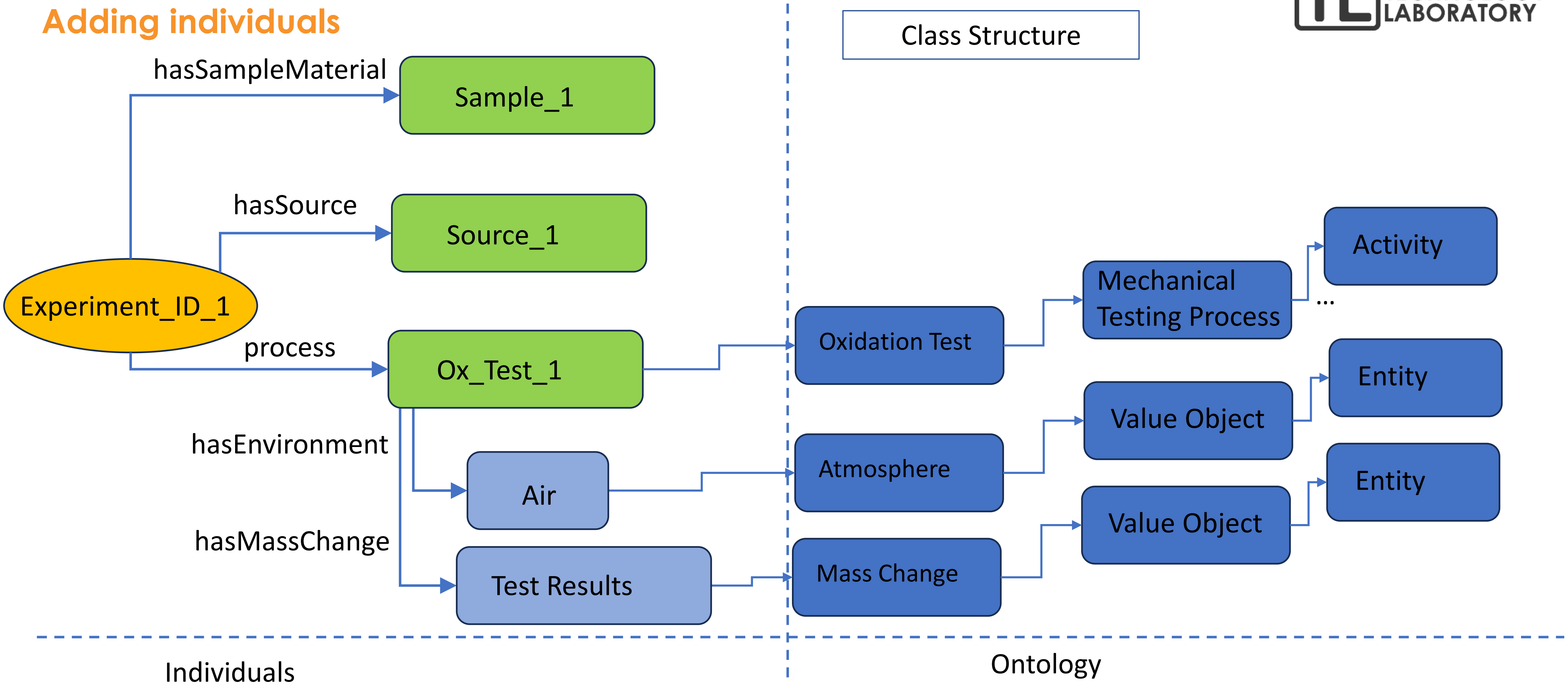
Representing Testing Data in the Ontology

Adding individuals



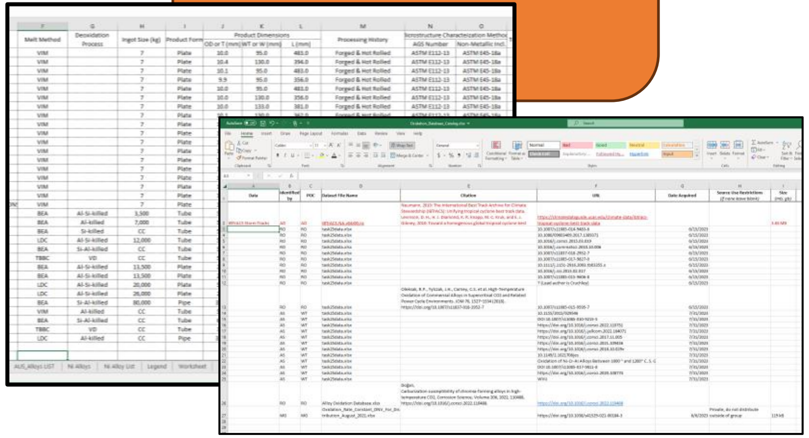
Representing Testing Data in the Ontology

Adding individuals



Leveraging the Ontology for Data Management

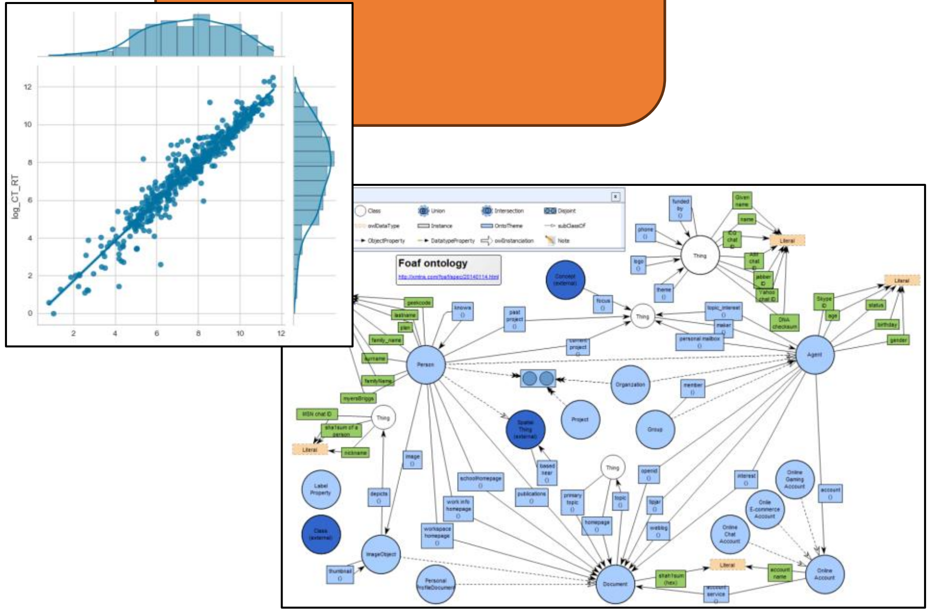
Local files



Internal Ontology + Database Structure

SPARQL Database

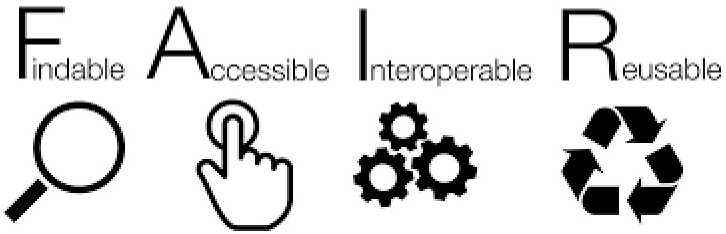
Data access & use



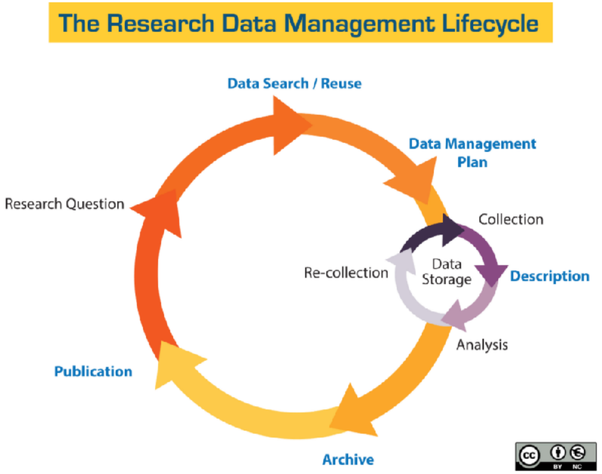
Benefits – Leveraging a Standard Materials Data Framework

Developing an ontology to underpin data management strategy

- Supports consistency across teams, projects, & work into the future
- Improvement in data reuse and knowledge retention
- Improved digitization to support data science & machine learning



- First step is to work towards standardizing the language used to identify the attributes; build in metadata
- Provides the basis for understanding the information and building connections between datasets



[Research data and FAIR - Research data management - All guides at RMIT University (libguides.com)]

Conclusion

- ✓ Generated a materials data ontology for alloy oxidation data
  - ✓ Building from existing domain upper-level ontology

- ✓ Captures complexity of attributes, relationships and metadata; standardized and structured for processes
  - ✓ Able to integrate with existing ontologies

- ✓ Capturing domain knowledge and machine-readable information for ensuring knowledge transfer, supporting advanced analytics

- ✓ Supporting standardization and reuse of data in research

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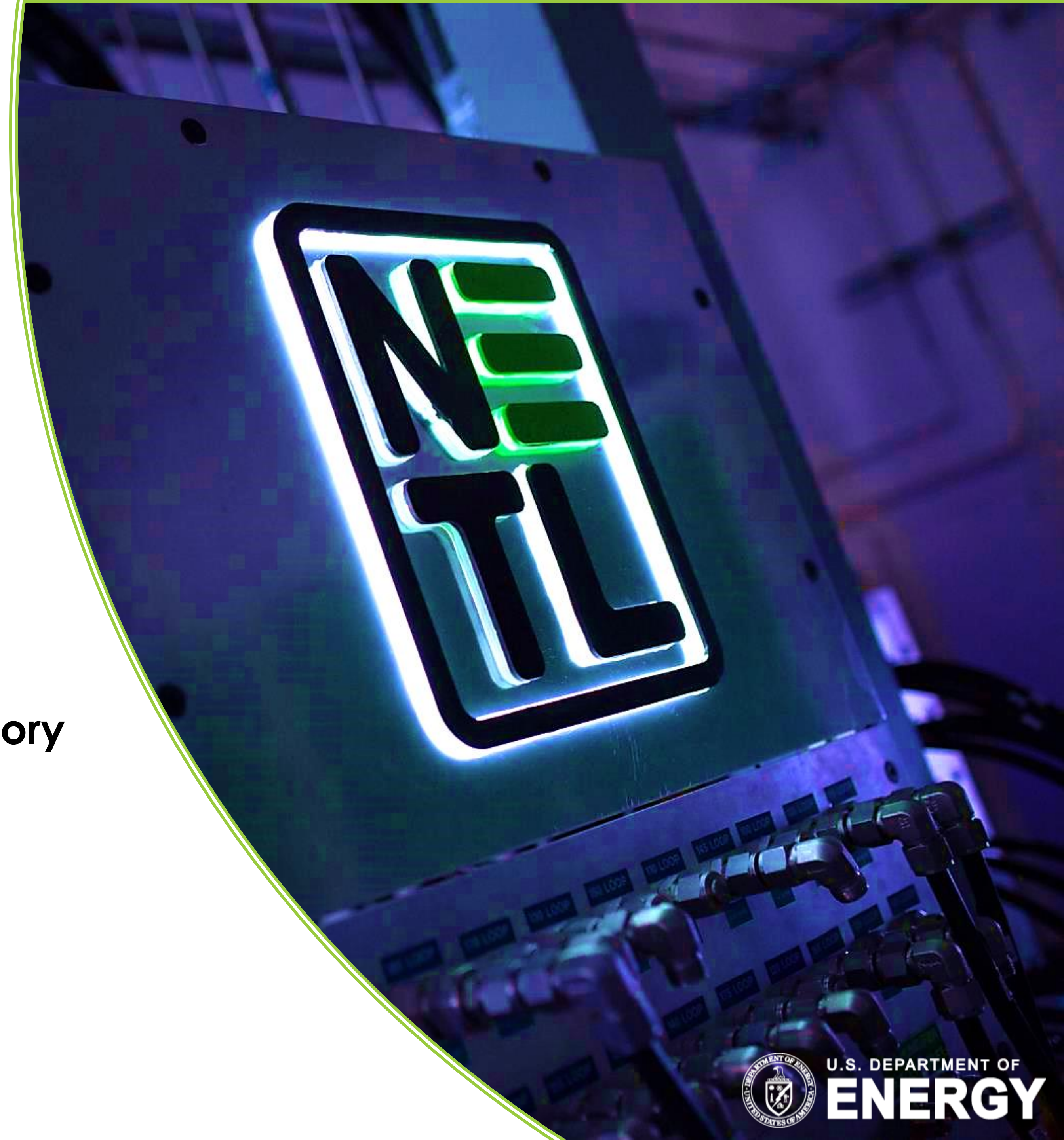

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