EMCC –Ontology and Data Management

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European Materials Characterization Council, Operational Management Board and Technical Project Advisors

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ON THE NEED FOR A DIGITAL REPRESENTATION OF MATERIALS DATA ALONG SCIENTIFIC AND INDUSTRIAL PROCESSES

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Introduction and own field of work

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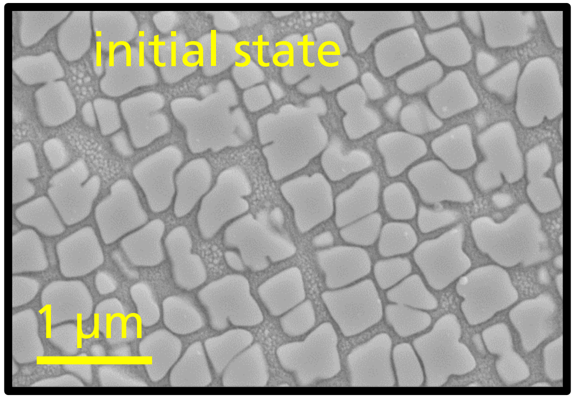
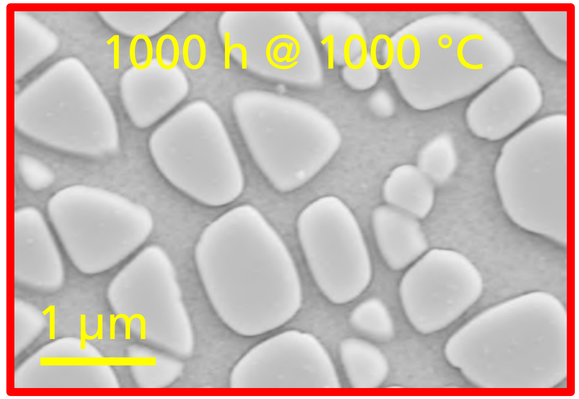
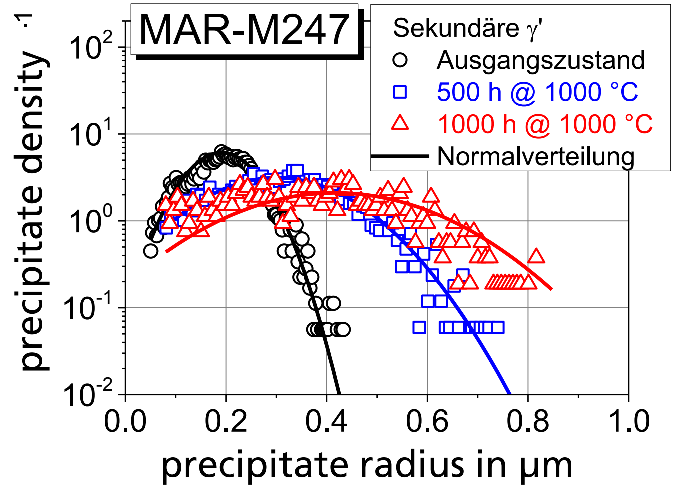
Introduction and own field of work

Systematic investigations and quantification of the evolution of precipitates for several nickel-base superalloys







- Aging of 8 superalloys at 800, 900 and 1000 °C up to 1000 h results in 120 material states
- Investigation of microstructure evolution using SEM
- Image processing & quantification of the trimodal γ' precipitate structure
- Accompanying mechanical tests, literature research on mechanical properties and thermodynamic simulations using MatCalc 6

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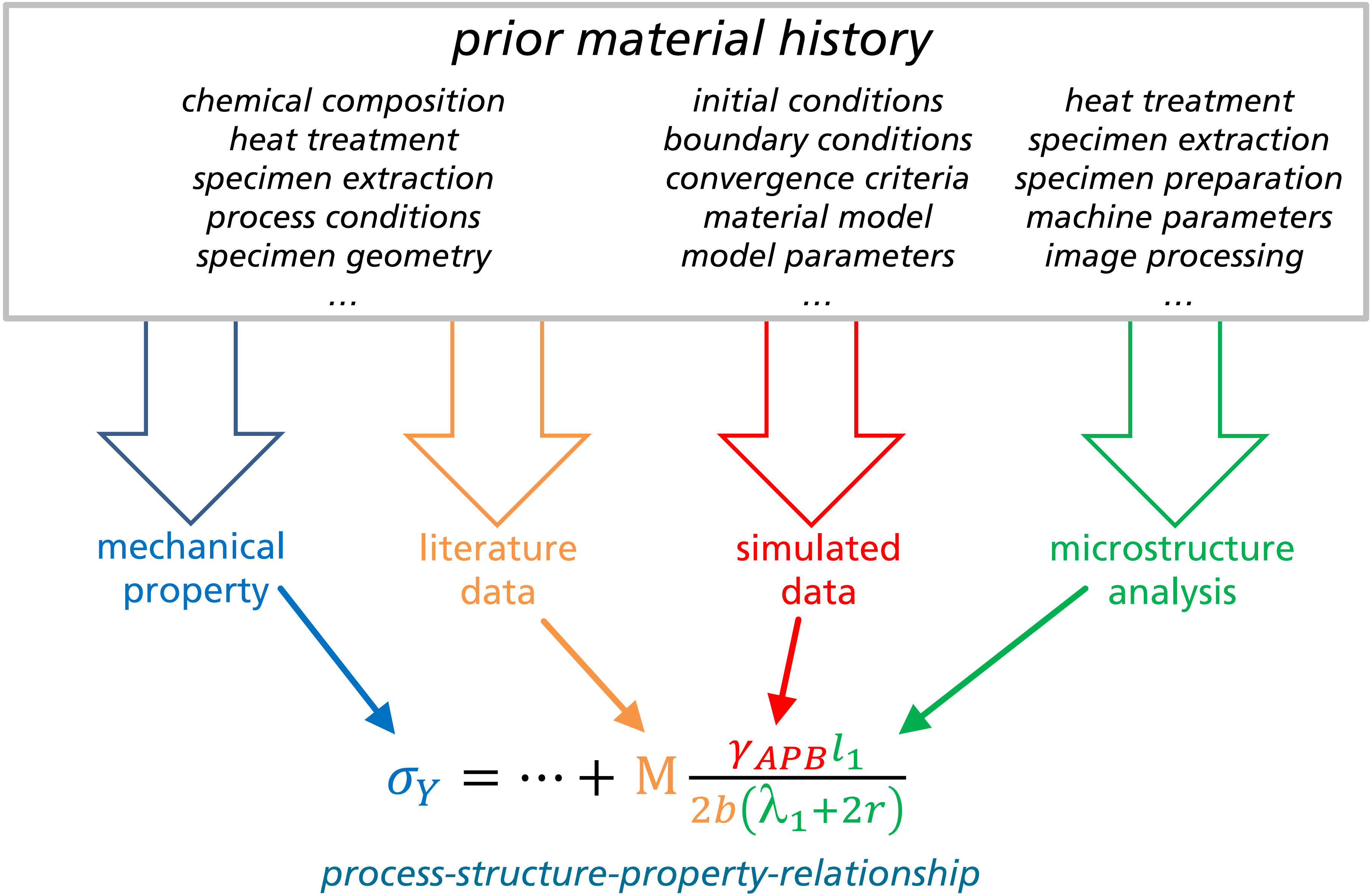
prior material history
chemical composition
heat treatment
specimen extraction
process conditions
specimen geometry
...
initial conditions
boundary conditions
convergence criteria
material model
model parameters
...
heat treatment
specimen extraction
specimen preparation
machine parameters
image processing
...
mechanical property
literature data
simulated data
microstructure analysis
$\sigma_Y = \cdots + M \frac{\gamma_{APB} l_1}{2b(\lambda_1+2r)}$
process-structure-property-relationship

Challenges

- The material history of a single specimen does not provide all information to obtain process-structure-property relationships
- Materials data is heterogeneous and contains lots of gaps
- Automatic data analysis requires strong semantics and a concept how to manage the materials data
- Research environment: A high degree of flexibility is required because
  - workflows,
  - processes,
  - research equipment,
  - analysis tools
  - data content change on a daily basis

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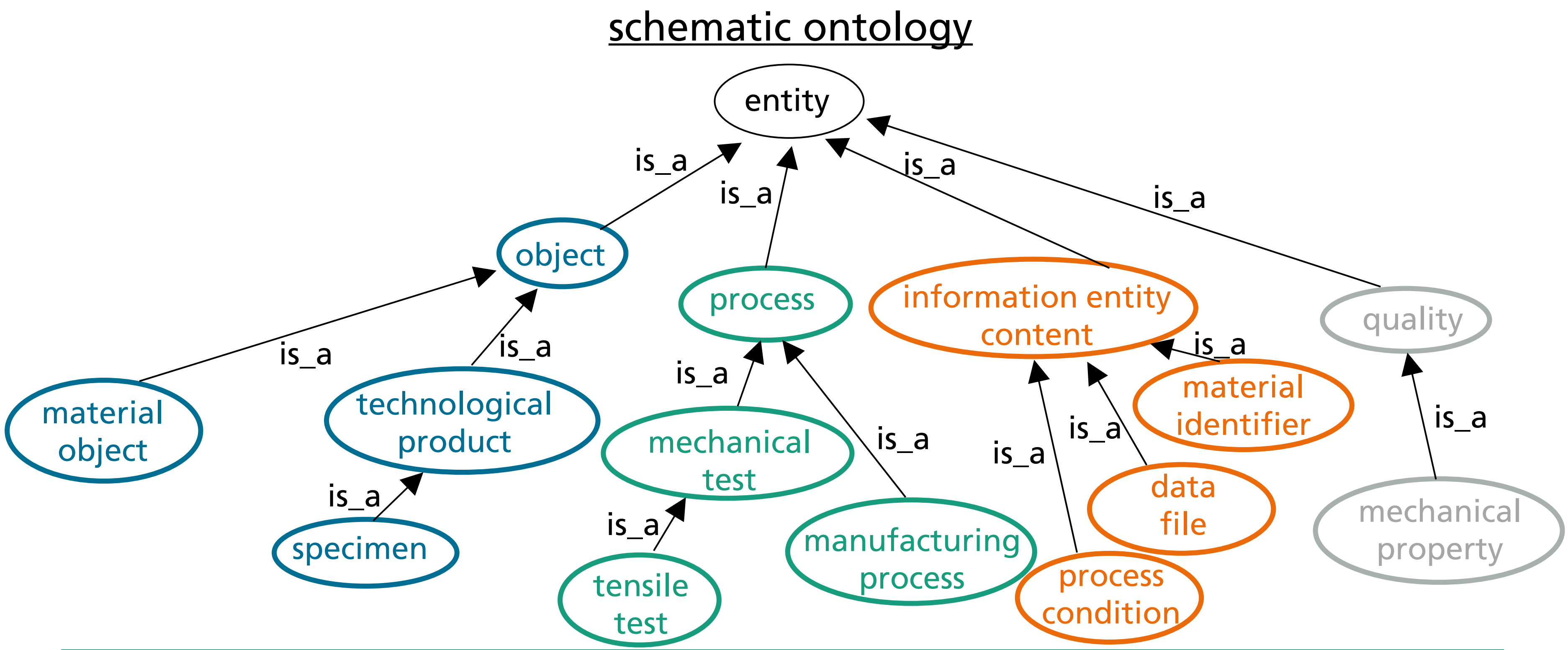
Directed network graph

Directed network graph

How to use an ontology to manage materials data within a network graph?



object process information entity content quality

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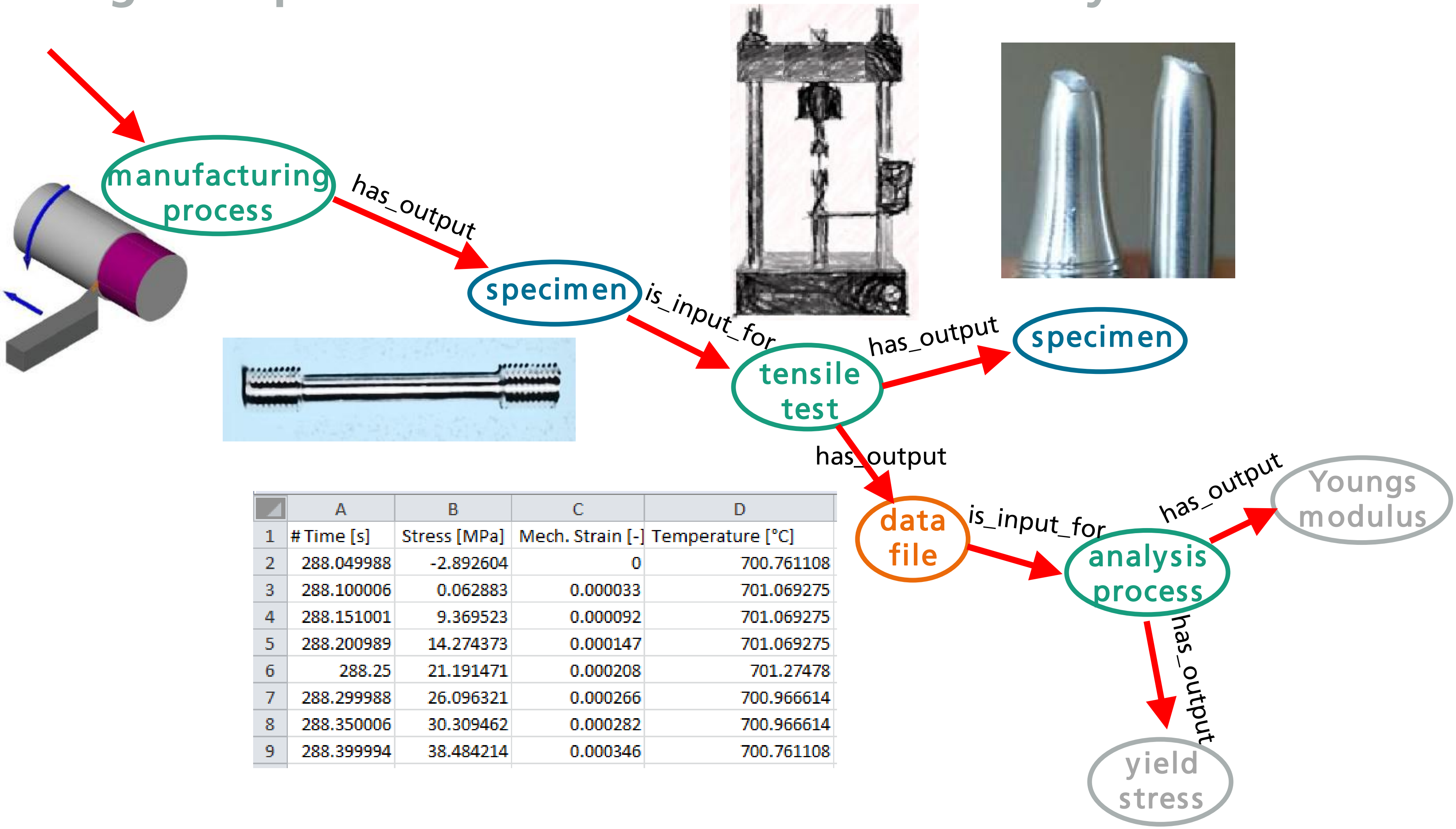
Directed network graph
Digital representation of the material history



	A	B	C	D
1	# Time [s]	Stress [MPa]	Mech. Strain [-]	Temperature [°C]
2	288.049988	-2.892604	0	700.761108
3	288.100006	0.062883	0.000033	701.069275
4	288.151001	9.369523	0.000092	701.069275
5	288.200989	14.274373	0.000147	701.069275
6	288.25	21.191471	0.000208	701.27478
7	288.299988	26.096321	0.000266	700.966614
8	288.350006	30.309462	0.000282	700.966614
9	288.399994	38.484214	0.000346	700.761108

object process information entity content quality

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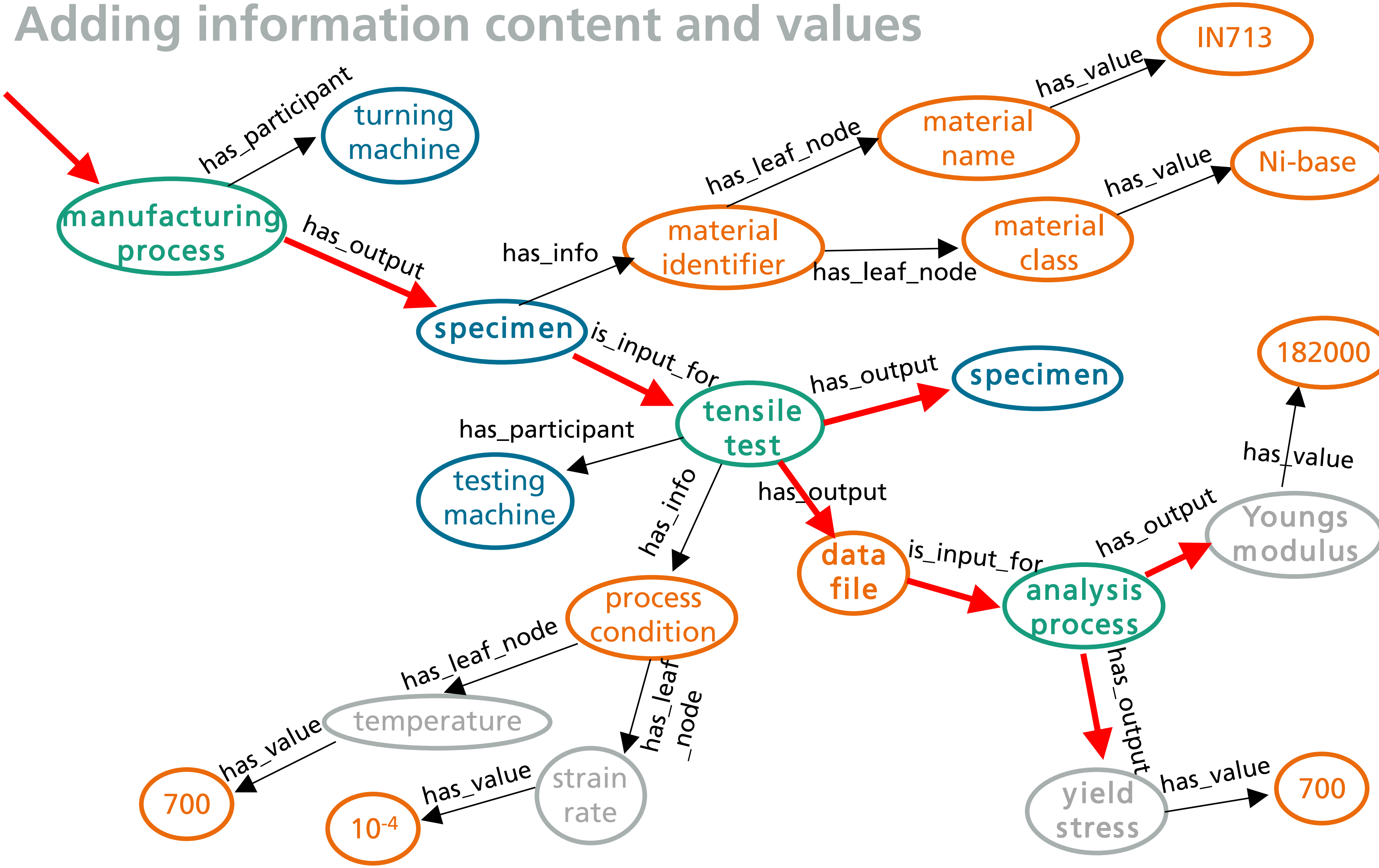
Directed network graph

Adding information content and values



object process information entity content quality

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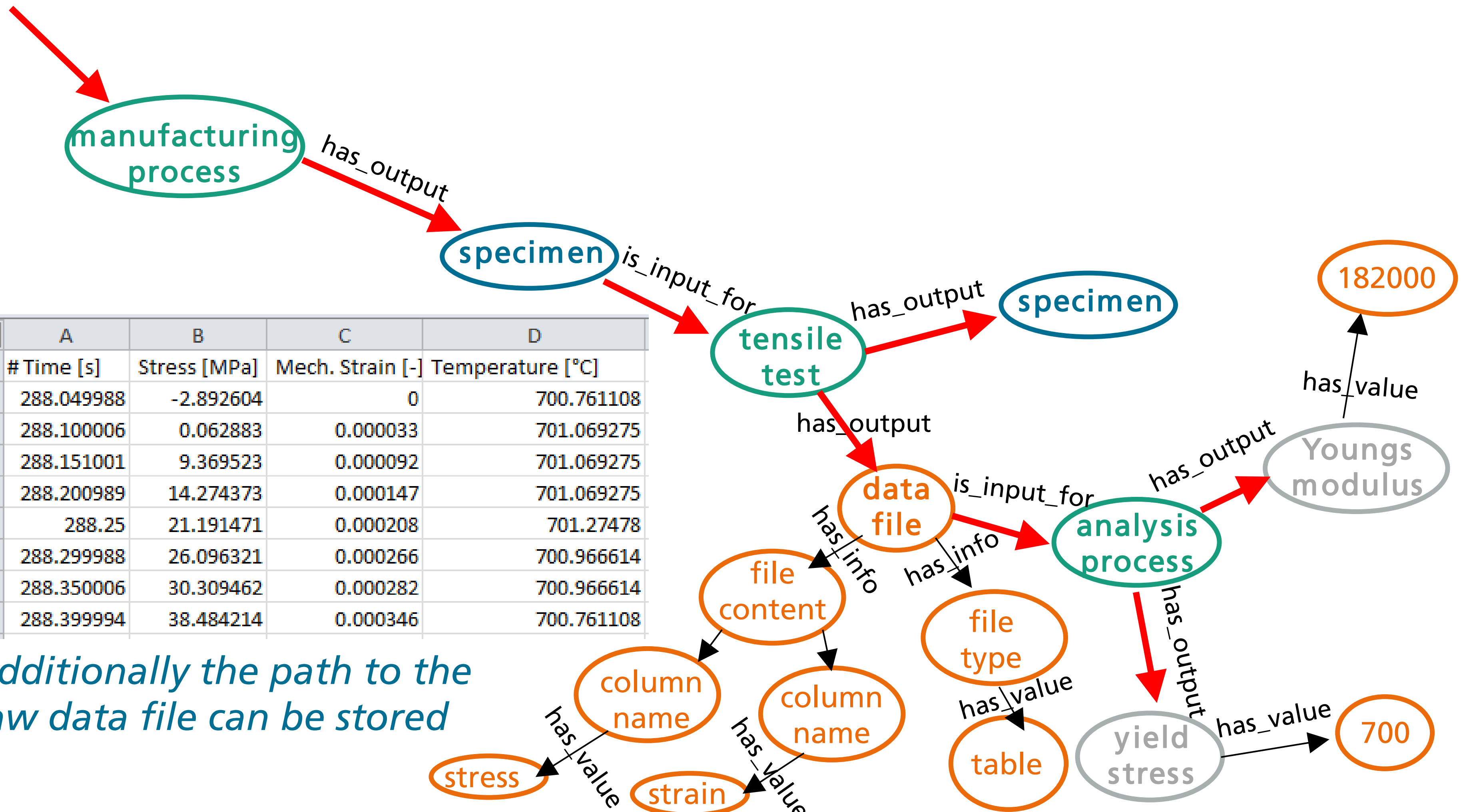
Directed network graph

Treatment of raw data files and its content



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Additionally the path to the raw data file can be stored

object process information entity content quality

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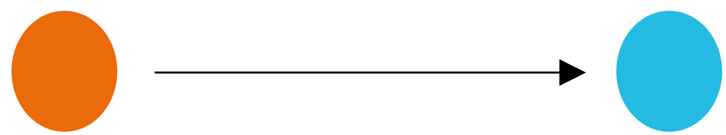
First steps towards an implementation

First steps towards an implementation
Management of the network graph

- SQL table to manage all nodes and relations from the network graph within a single table



<u>table row:</u> *source node (ID & type)* *relation (ID & type)* *target node (ID & type)*

Filtering and finding nodes and relations
is very simple and efficient

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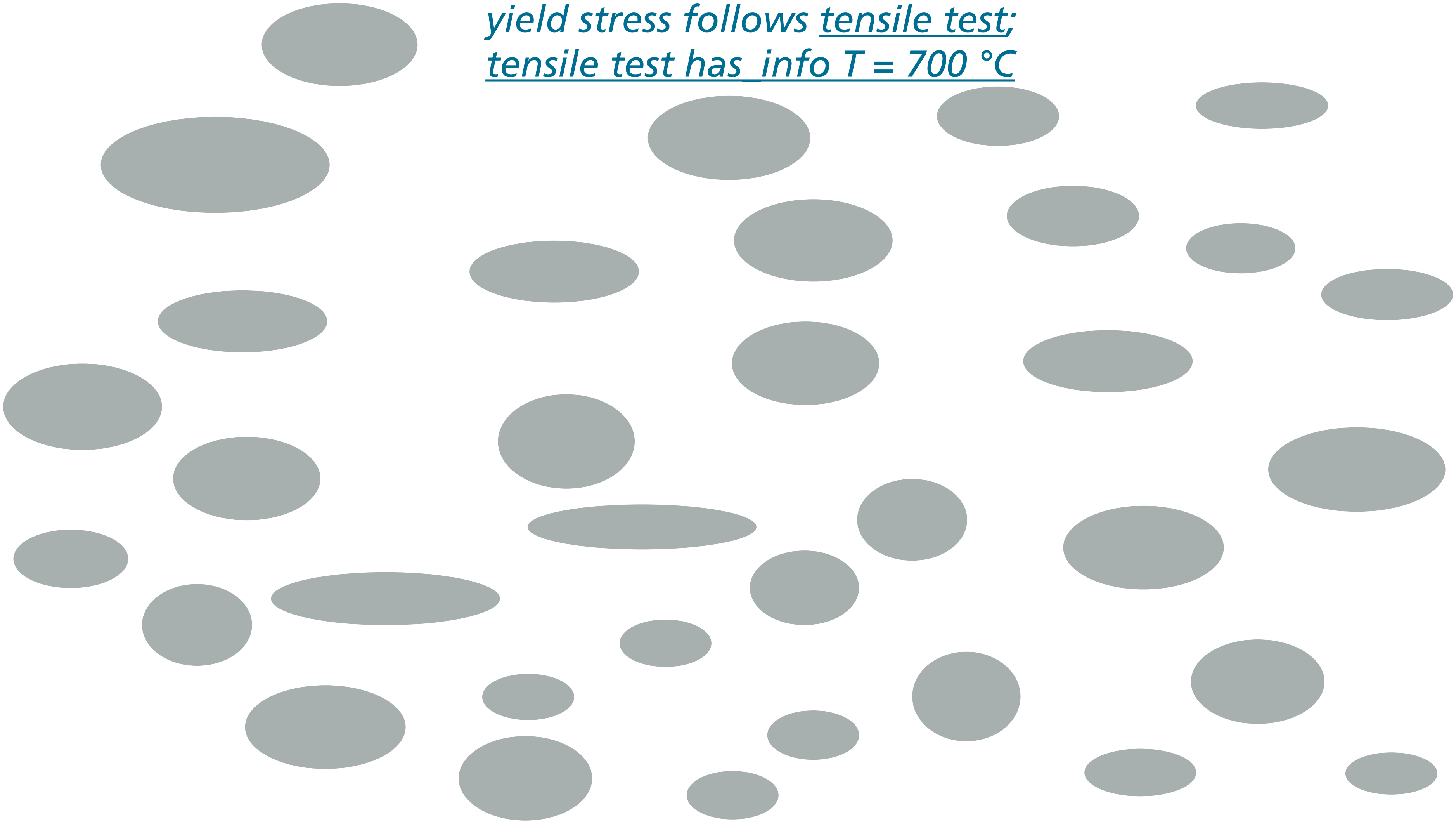
Implementation

Query:

Find all yield stress values for material name IN713;
yield stress follows tensile test;
tensile test has_info T = 700 °C



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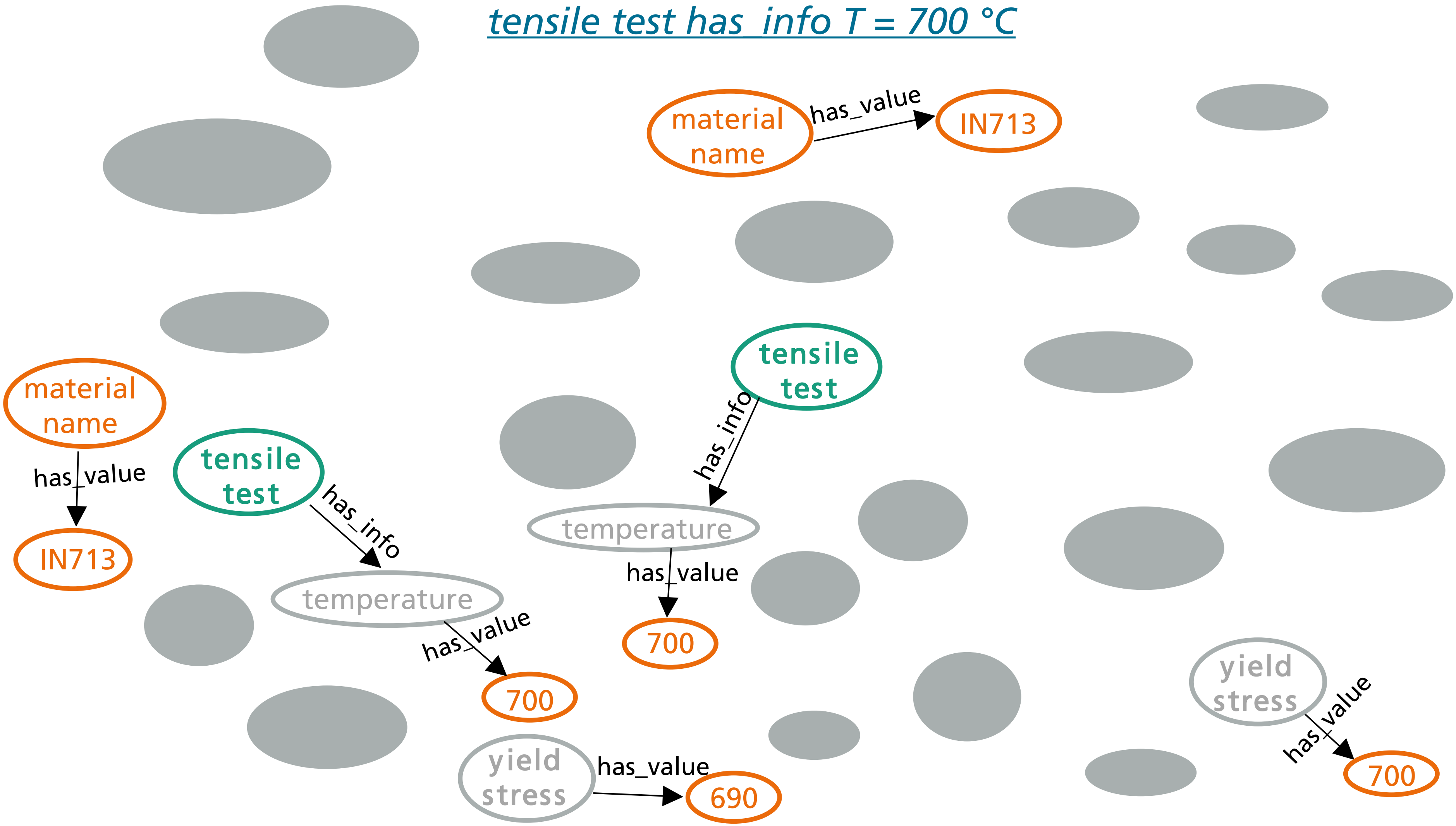
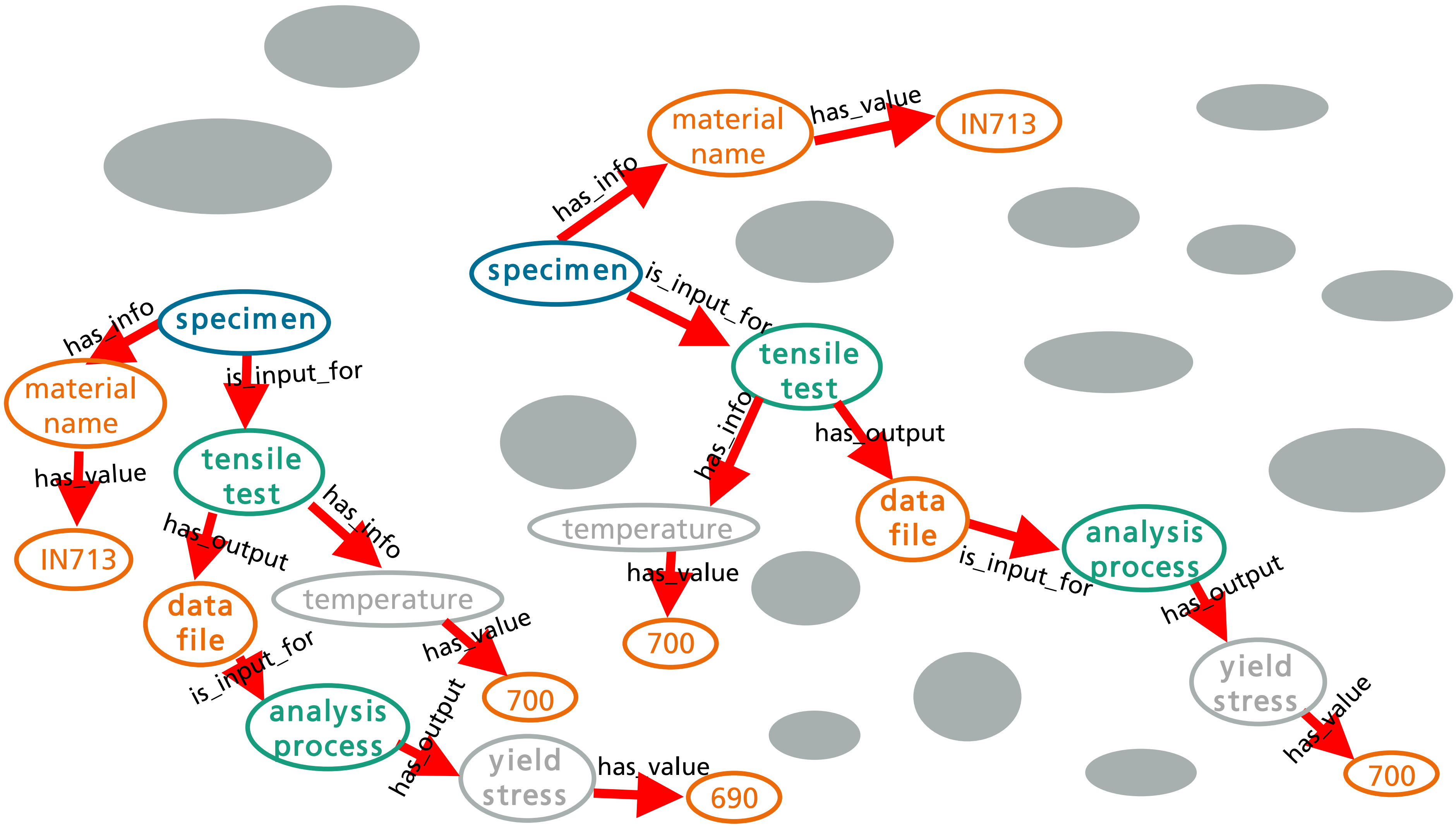
Implementation

Query: *Find all yield stress values for material name IN713; yield stress follows tensile test; tensile test has_info T = 700 °C*



Implementation

The query only delivers a hit, if the information is connected through the same branch.



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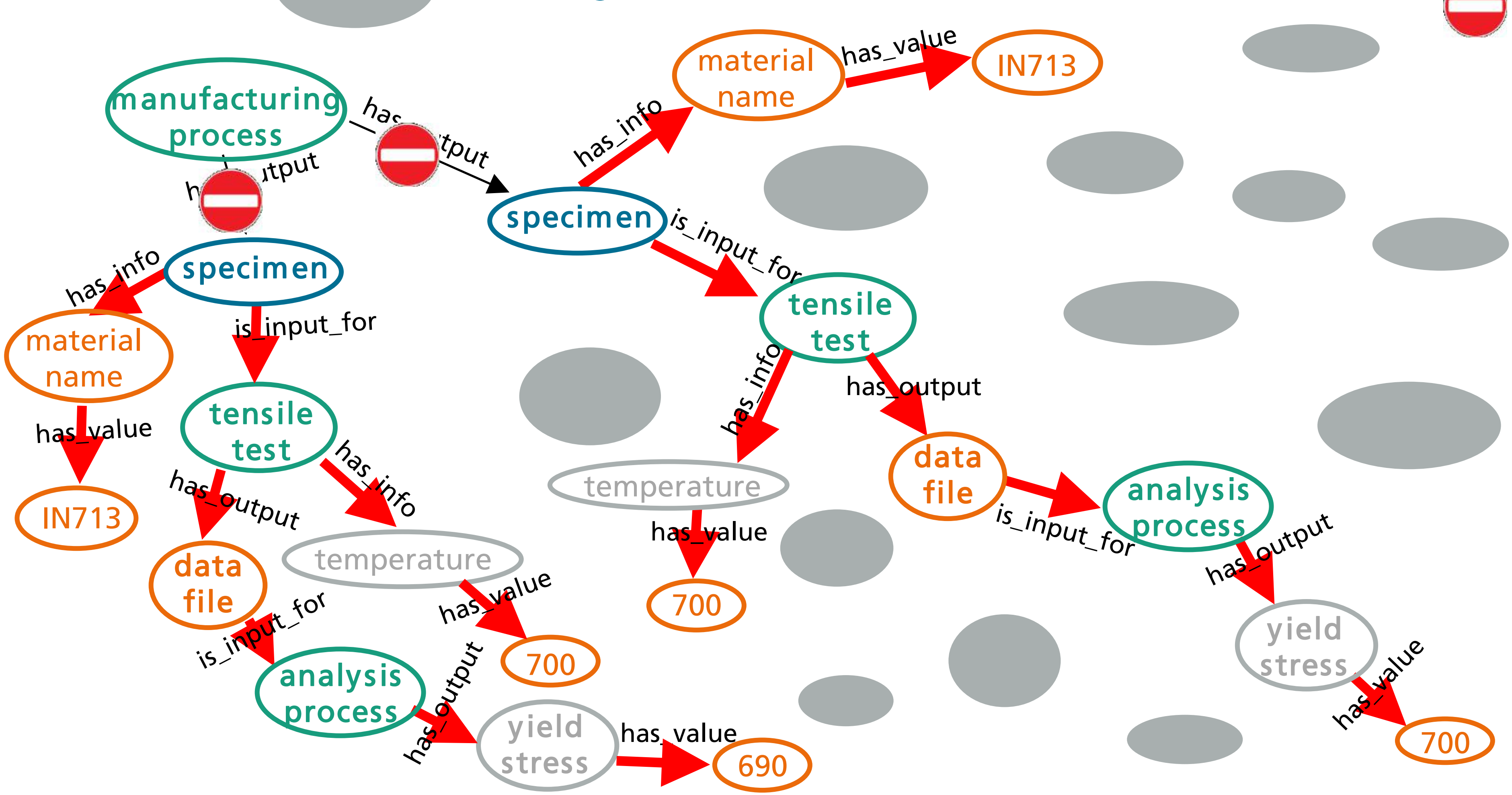
Implementation

The query only delivers a hit, if the information is connected through the same branch.

Unlogical crosslinks need to be excluded!



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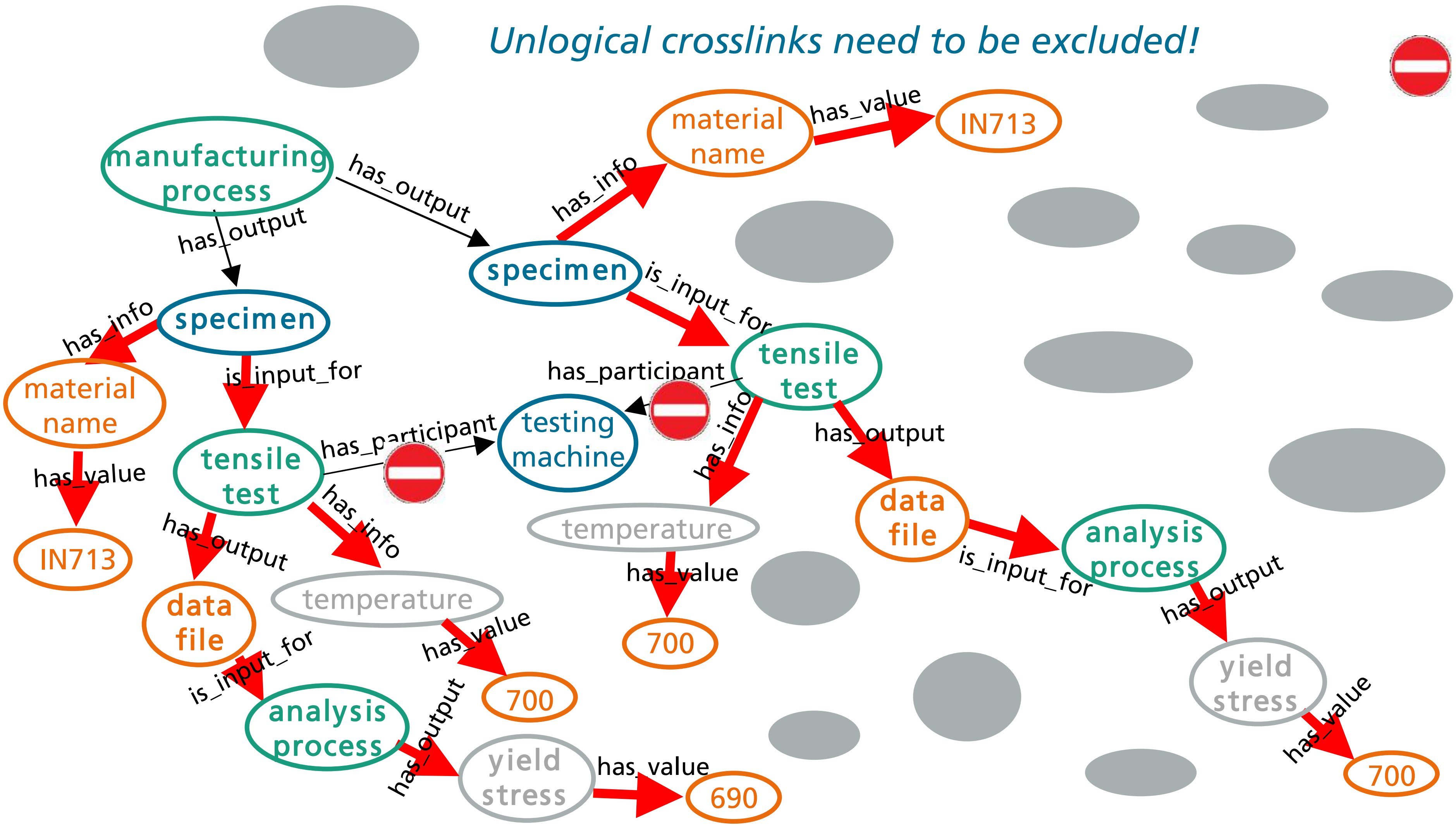

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Implementation

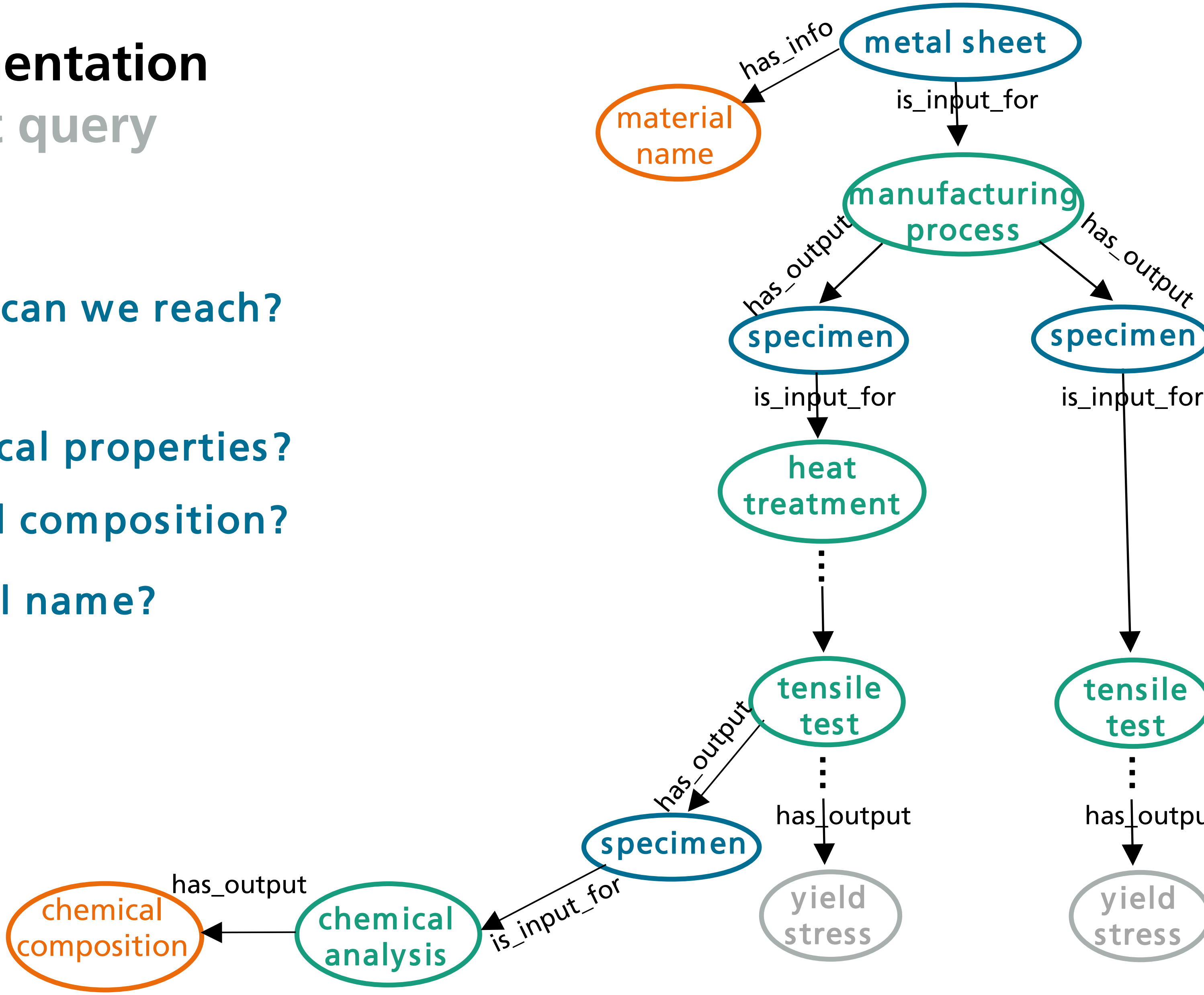
Default query

How far can we reach?

Mechanical properties?

Chemical composition?

Technical name?



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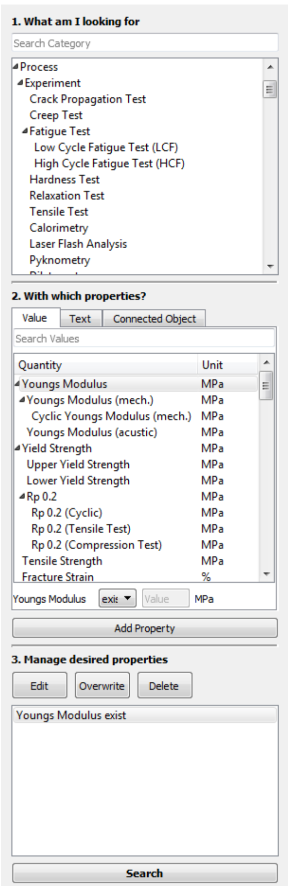
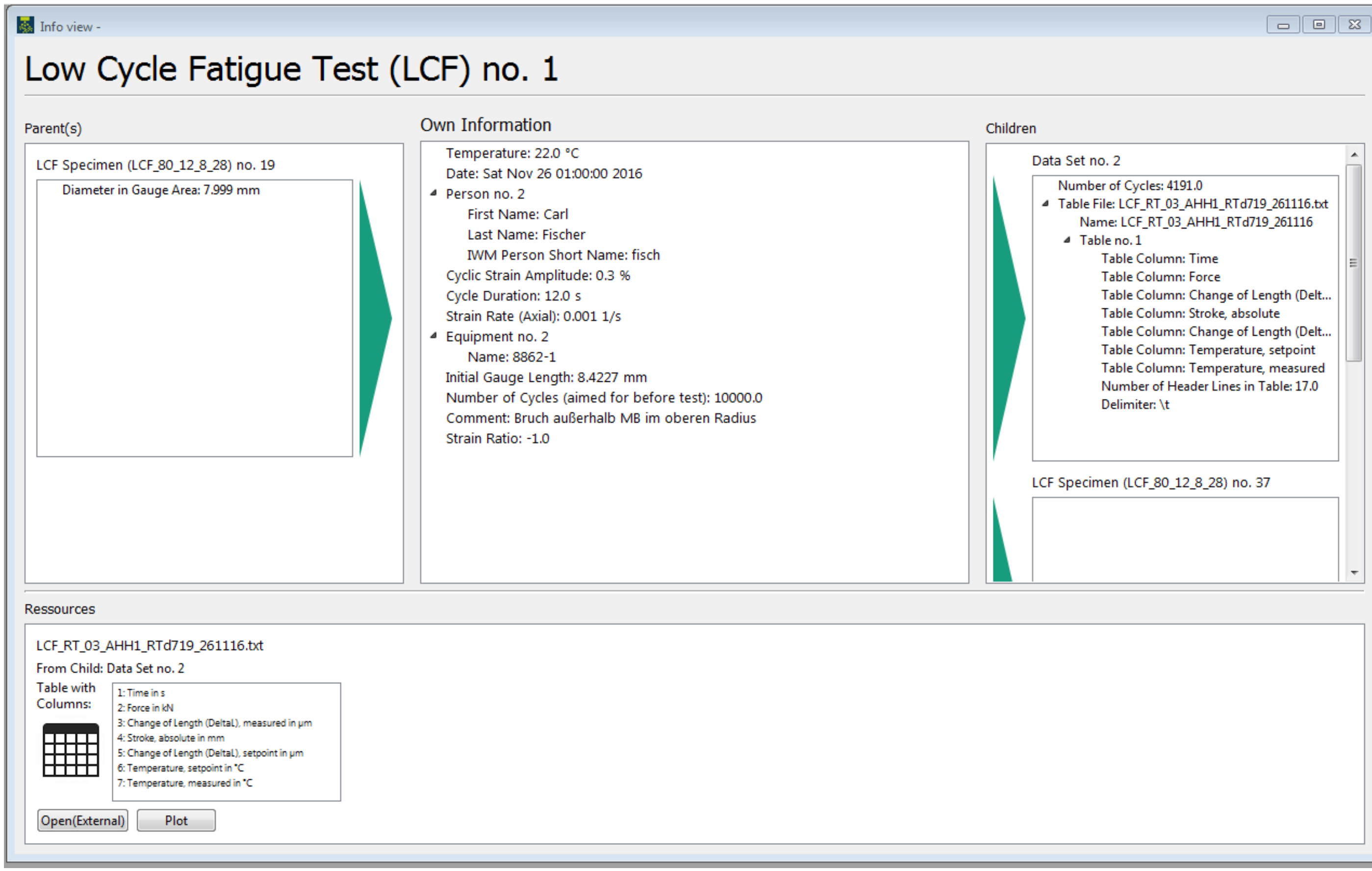
First Software Implementation

First Software Implementation

Combinatorial search through ontology

Backtracking materials history including visualization of raw data





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