

# ONTOLOGY AND WHY CONTEXT MATTERS

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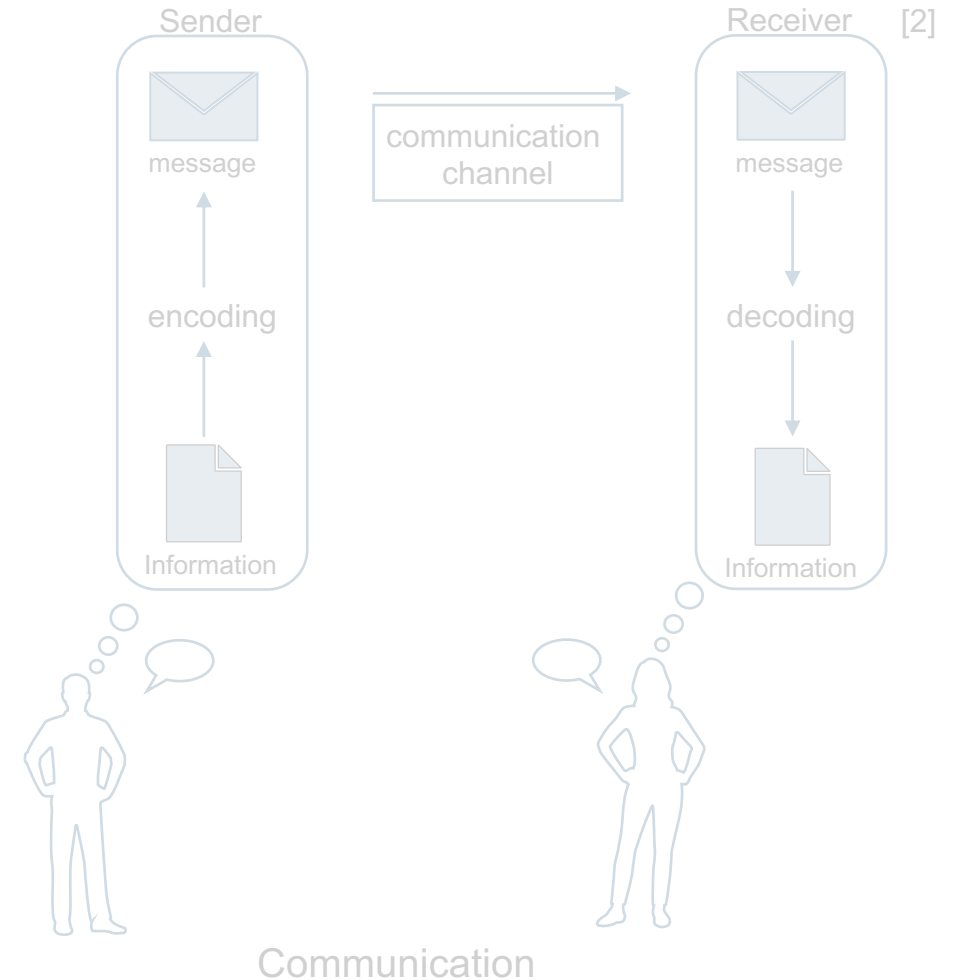
MSE Day, Hereon Geesthacht, 14.11.2023

# MOTIVATION

## LANGUAGE AND COMMUNICATION

- Language can be used to **represent knowledge**.
- What is Language?
  - System of conventional **spoken, manual, or written symbols** combined to **convey meaning** [1].
  - Language is used by human beings to **express** themselves.
- **Communication** is one of the functions of language
- Successful communication depends on:
  - Information has to be correctly **encoded** via **syntax**.
  - The meaning (**semantics**) of the encoded information must be interpreted correctly (**understanding**).
  - The **understanding or decoding** process is influenced by the **context** of sender and receiver

[1] <https://www.britannica.com/topic/language>  
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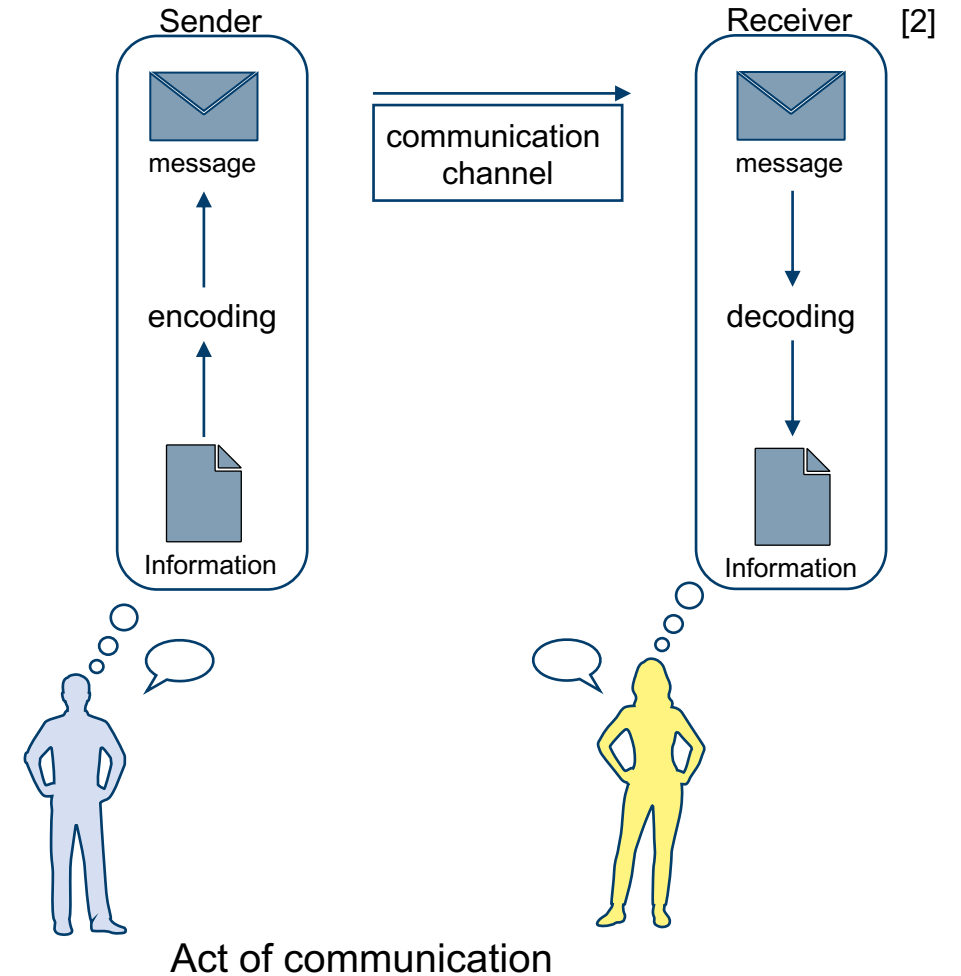
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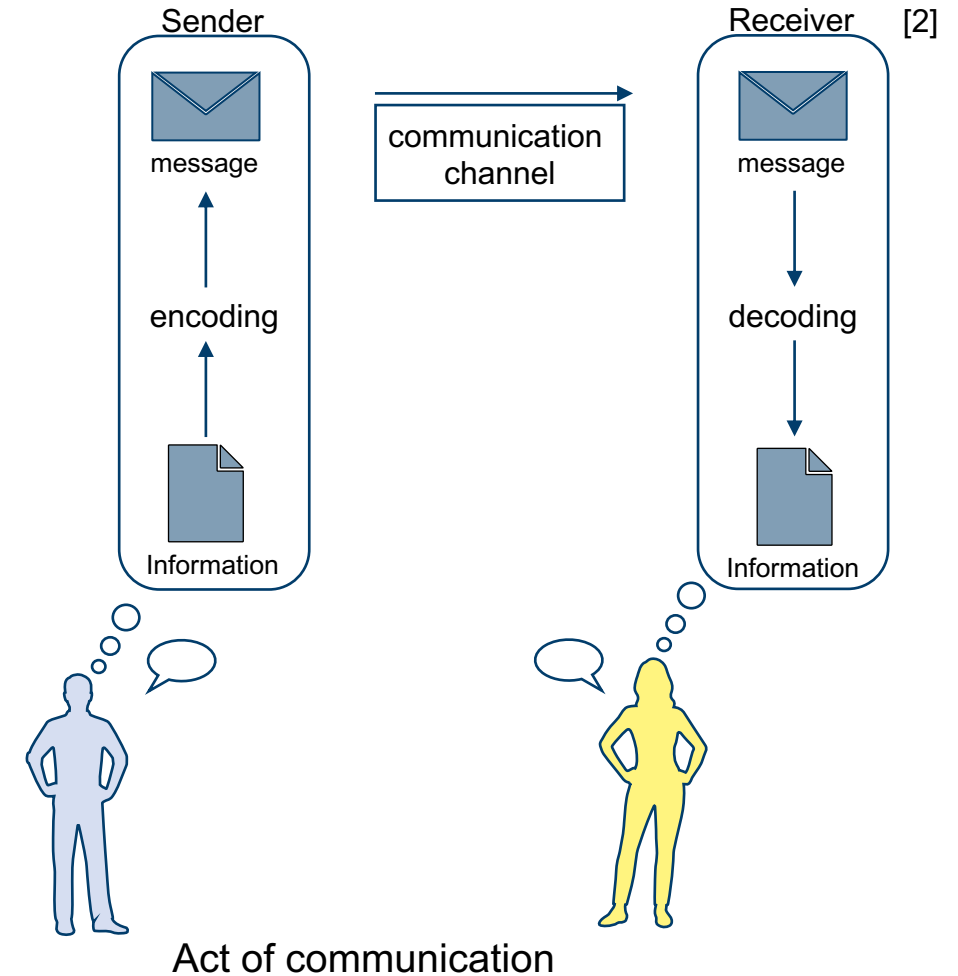
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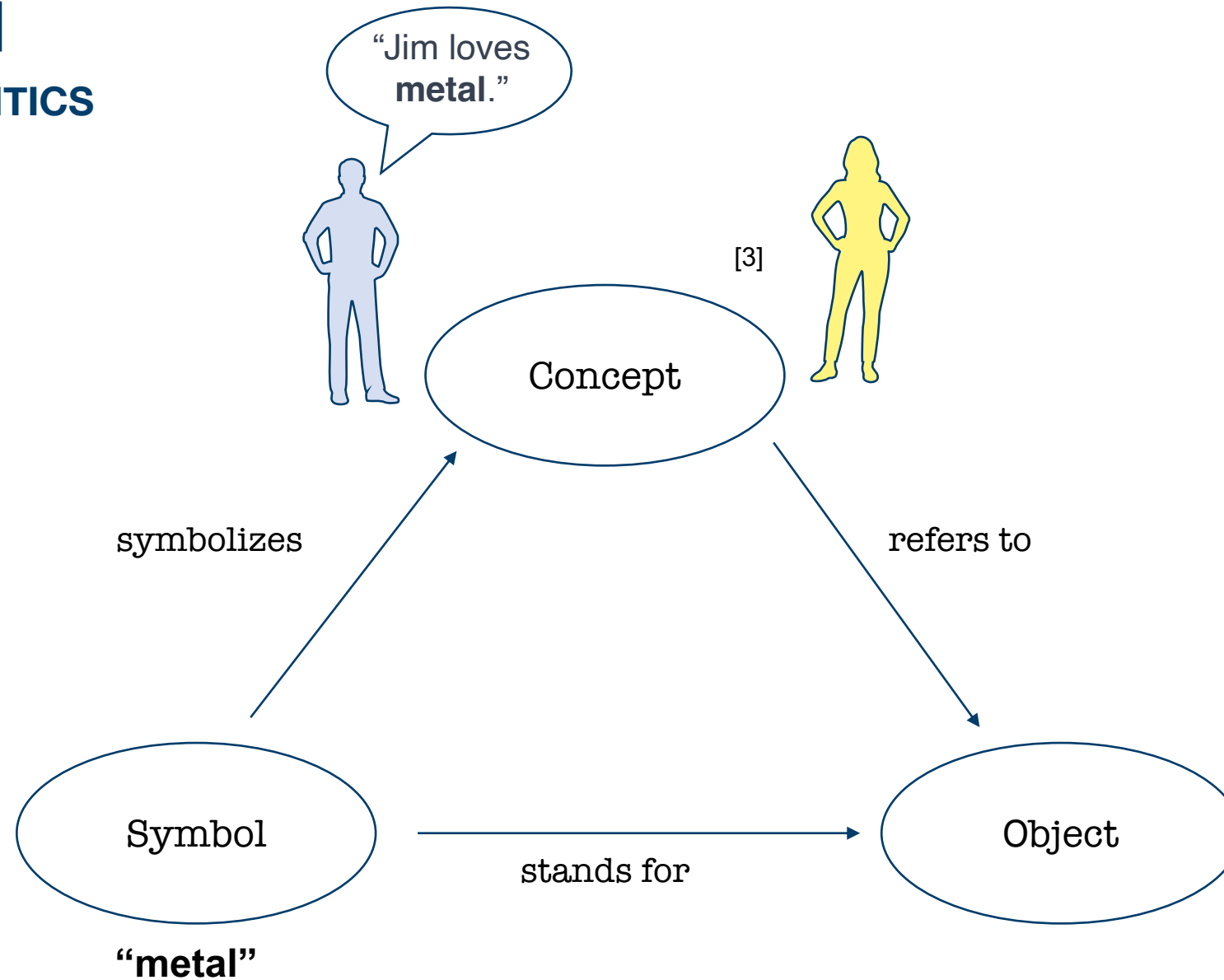
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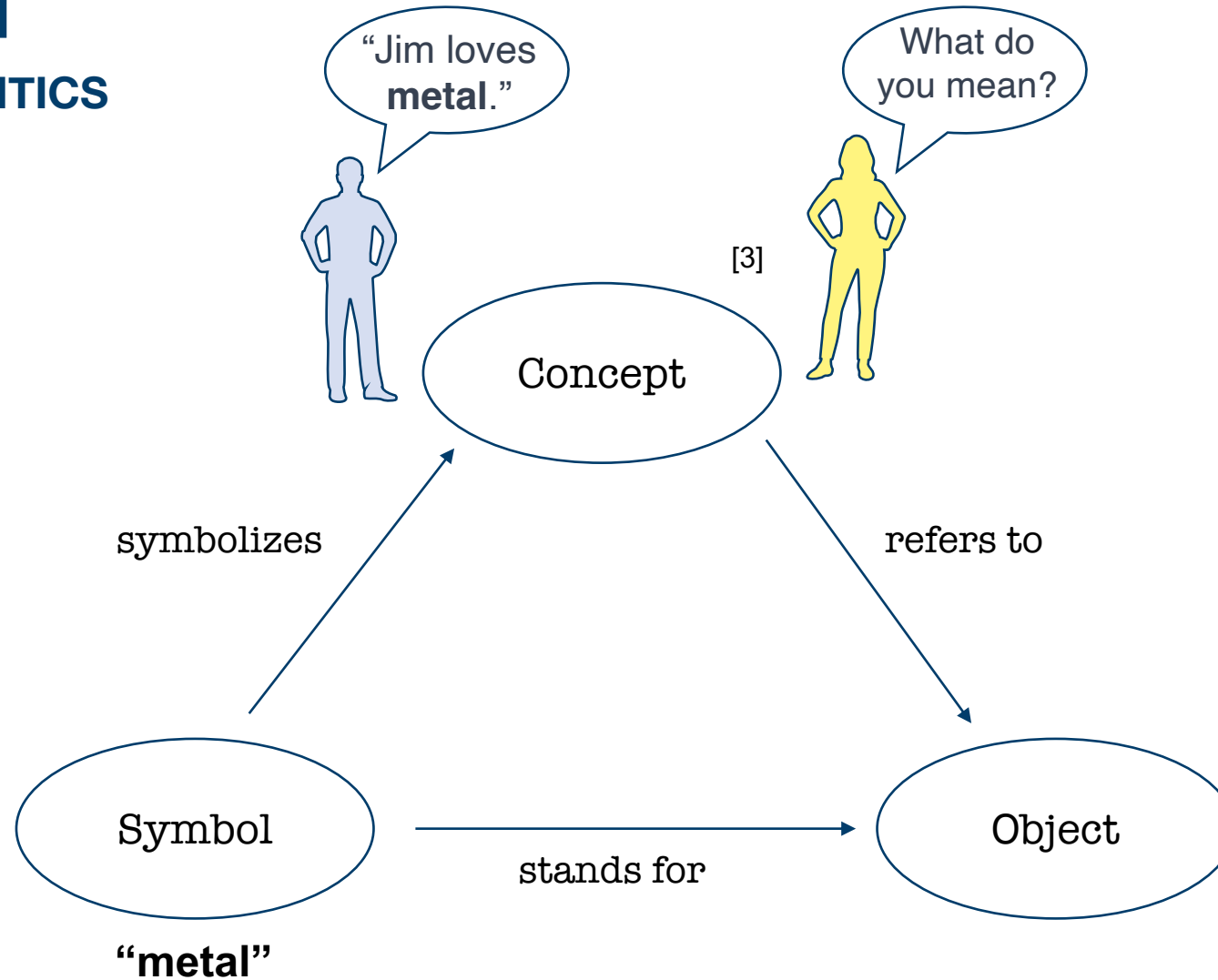
# MOTIVATION

## CONTEXT AND SEMANTICS

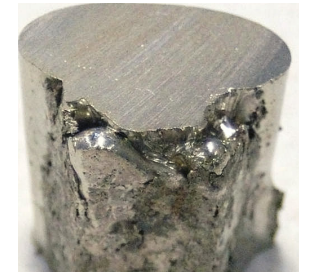


# MOTIVATION

## CONTEXT AND SEMANTICS



Music(Metal)



Material(Metal)



Software(Metal)

[3] C. K. Ogden and I. A. Richards (1923) The Meaning of Meaning

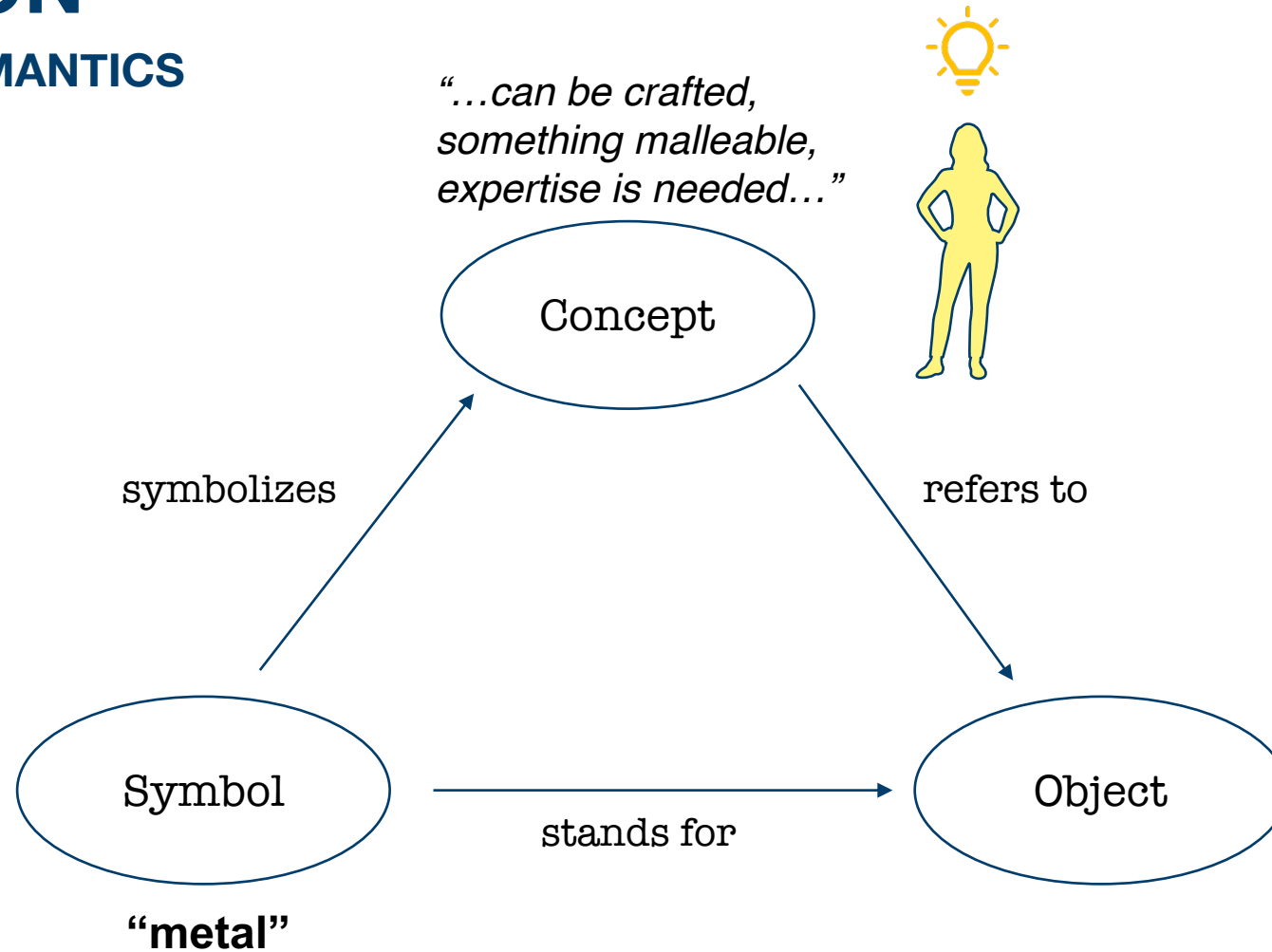
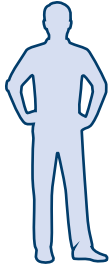
[4] <https://en.wikipedia.org/wiki/Nickel>

[5] <https://developer.apple.com/metal/>

# MOTIVATION

## CONTEXT AND SEMANTICS

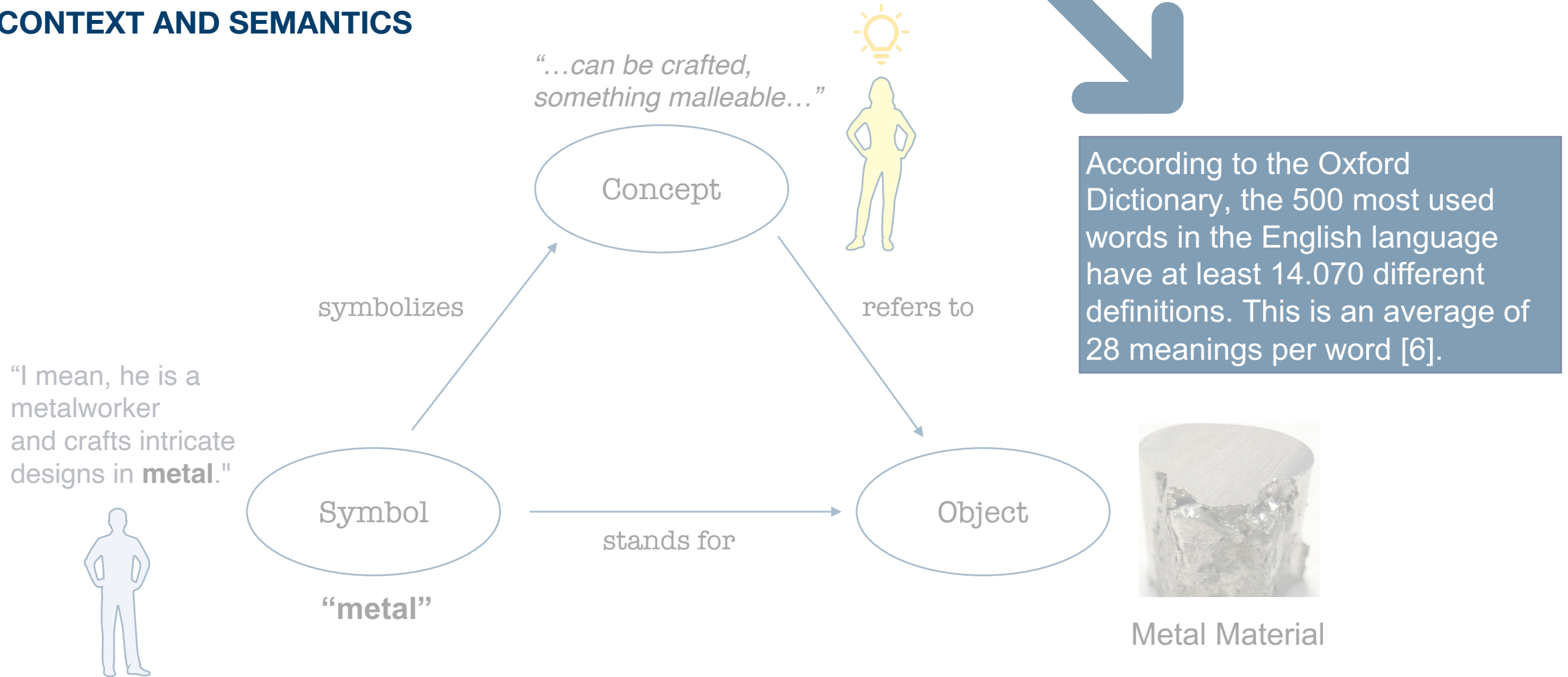
“I mean, he is a metalworker and crafts intricate designs using the medium of **metal**.”



Metal Material

# MOTIVATION

## CONTEXT AND SEMANTICS



[6] <http://inmyownterms.com/mysmarterms/mysmarterms-5-the-semantic-triangle-words-dont-mean-people-mean/>



# MOTIVATION

## FORMAL KNOWLEDGE REPRESENTATION

- Formal knowledge representation:
  - It is a field of AI.
  - It unambiguously captures the **semantics** of **concepts, properties, relationships**, and **entities**.
  - These semantics relates to specific **knowledge of domains**, i.e., fields of interest or areas of concern.
- **Machines (computers)** must be able to **understand** knowledge representations

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# FAIR

## To be interoperable...

- I1. (meta)data use a **formal**, accessible, shared, and broadly applicable **language for knowledge representation**.
- I2. (meta)data use vocabularies that follow FAIR principles.
- I3. (meta)data include qualified references to other (meta)data.

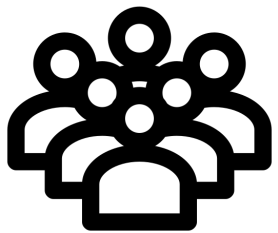
# ONTOLOGY

## WHAT IS ONTOLOGY?

An ontology is an **explicit, formal specification of a shared conceptualization** [7].

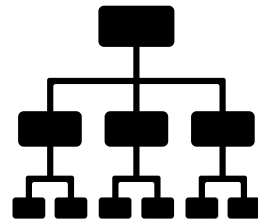
### Shared

Reach consensus  
(shared understanding)  
about ontology.



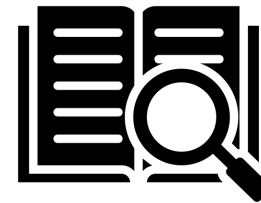
### Conceptualization

Abstract model about  
specific domain.



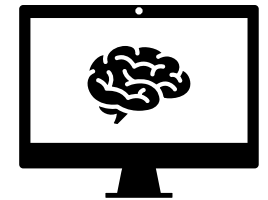
### Explicit

Meaning of all concepts  
must be defined.



### Formal

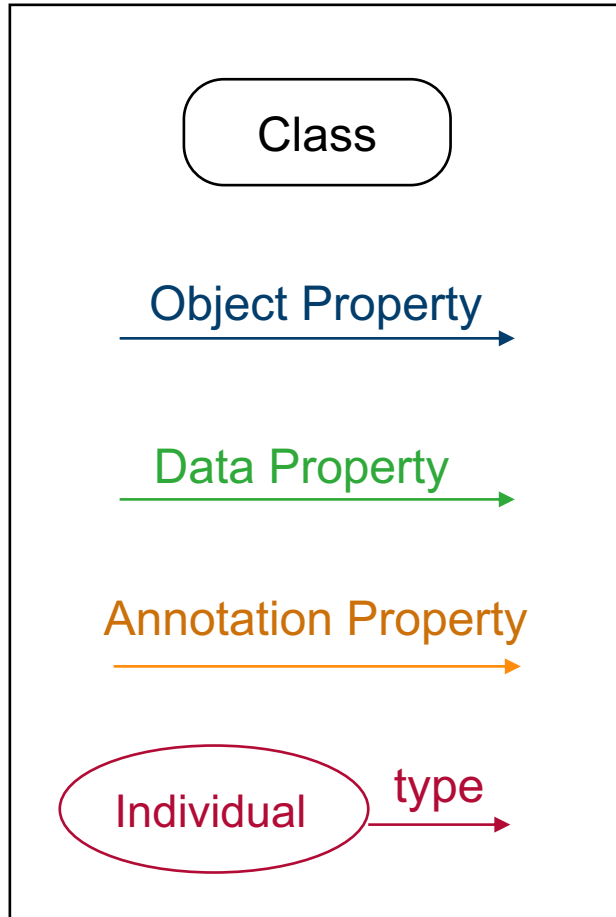
Machine  
understandable.



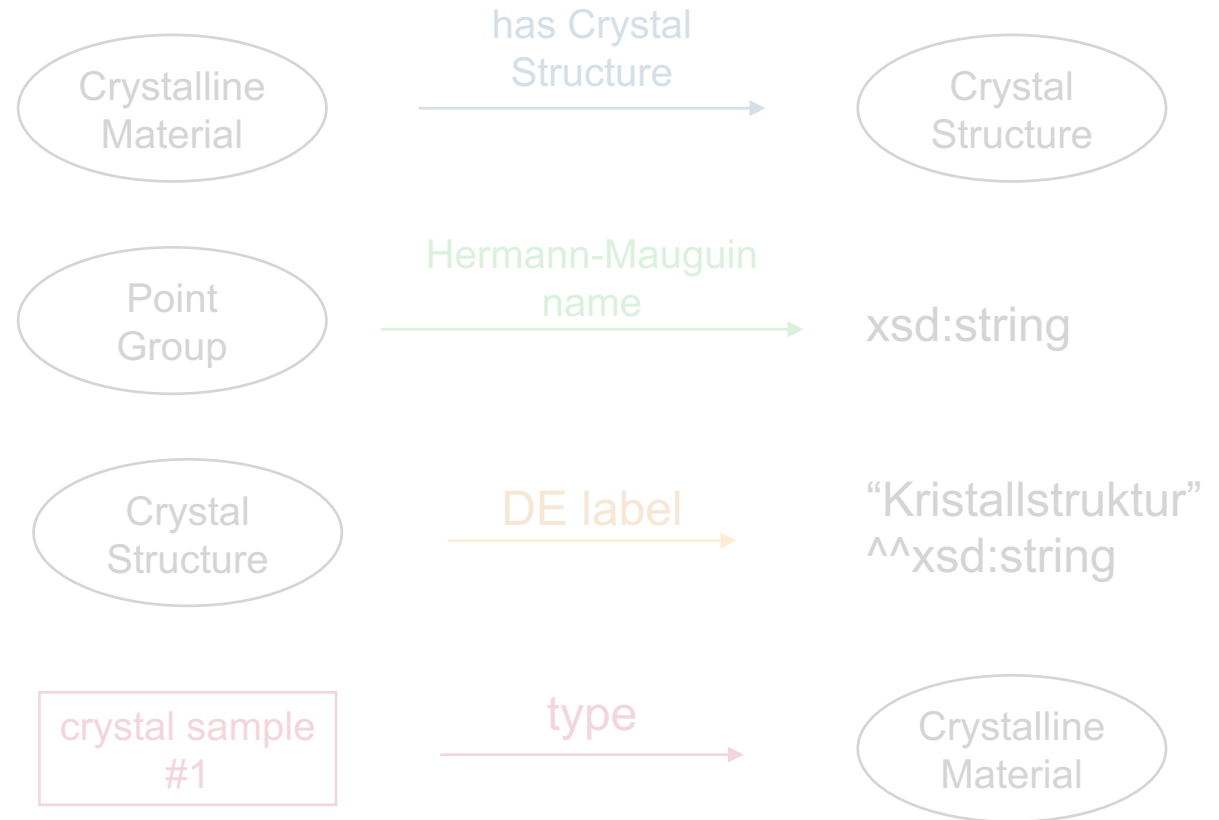
# ONTOLOGY

## HOW TO REPRESENT ONTOLOGY (1)

### Ontology Entities



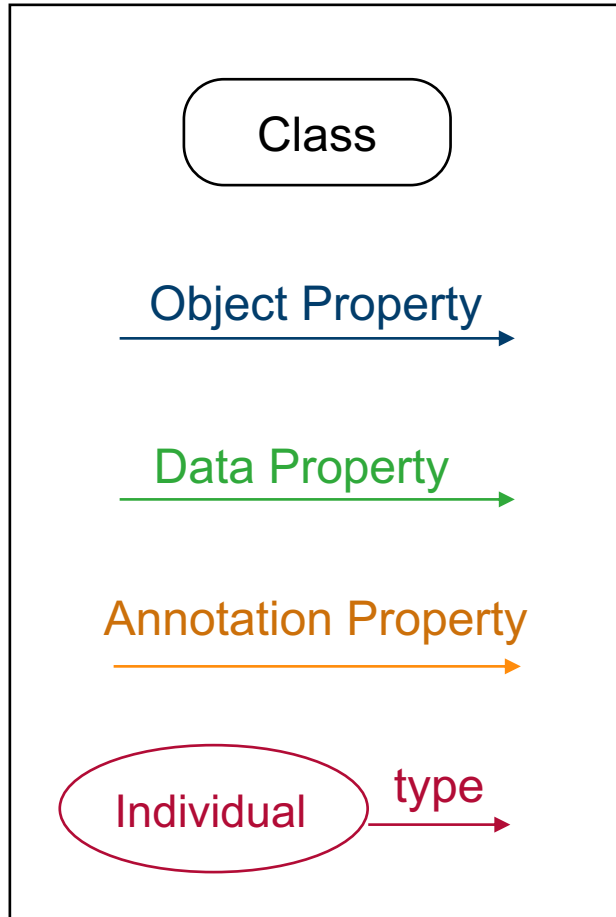
### Example



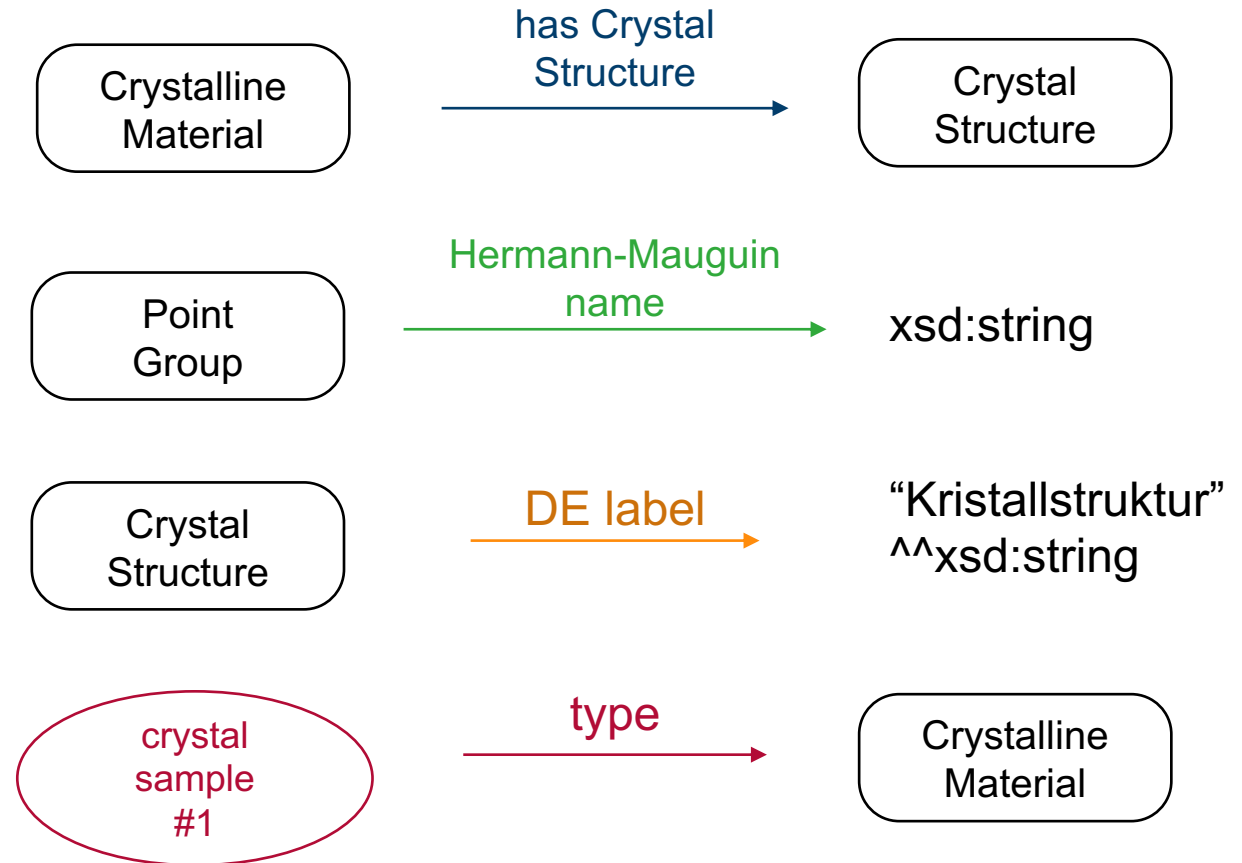
# ONTOLOGY

## HOW TO REPRESENT ONTOLOGY (2)

### Ontology Entities



### Example



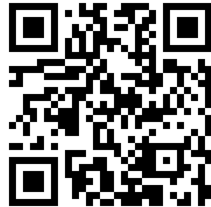
# ONTOLOGY APPLICATIONS

## CRYSTALLOGRAPHIC DEFECT ONTOLOGY

- **Crystal Defect Ontology (CDO)**: harmonized understanding & description of crystal defect across
  - scales (nano/micro/meso),
  - dimensions (0D-3D), and
  - methods (simulations & experiments)



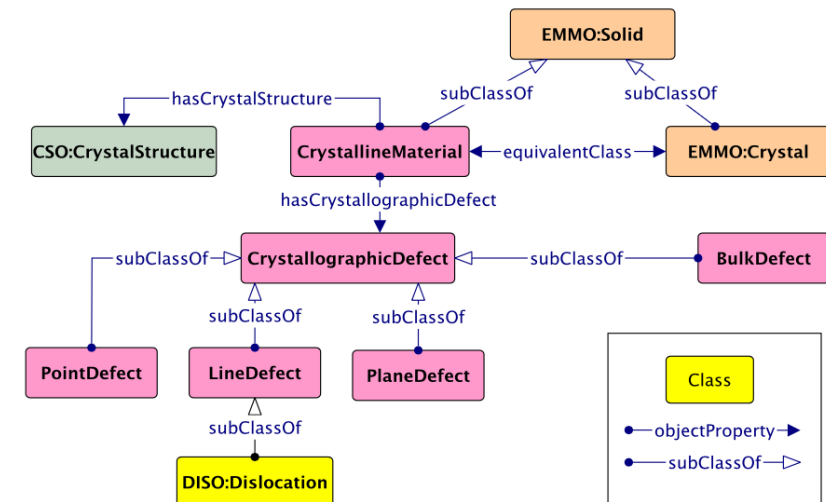
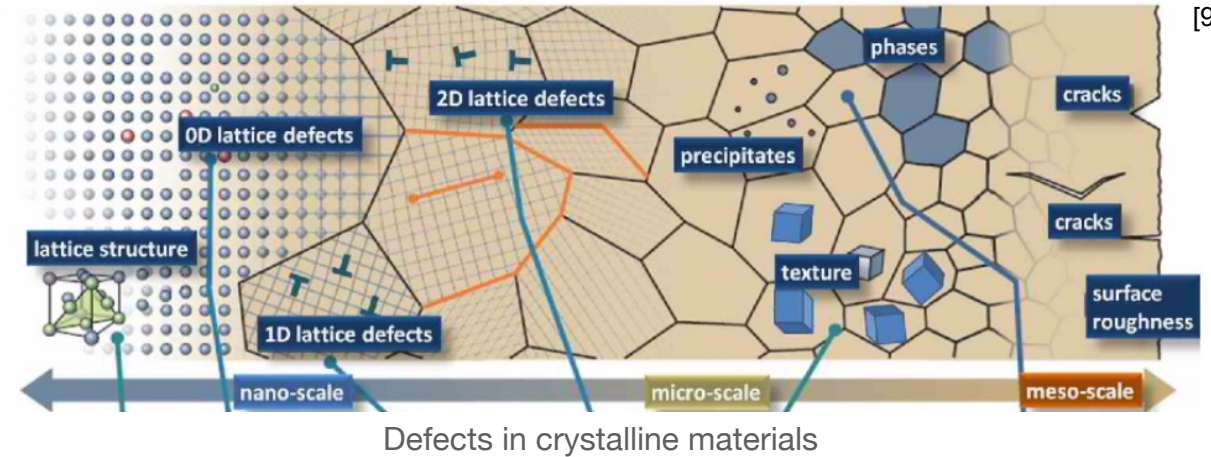
Crystallographic Defect Ontology



Dislocation Ontology



Planar and Point Defect Ontology



Crystallographic Defect Ontology

AZ Ihsan, AA Guzman, S Fathalla, V Hofmann, S Sandfeld

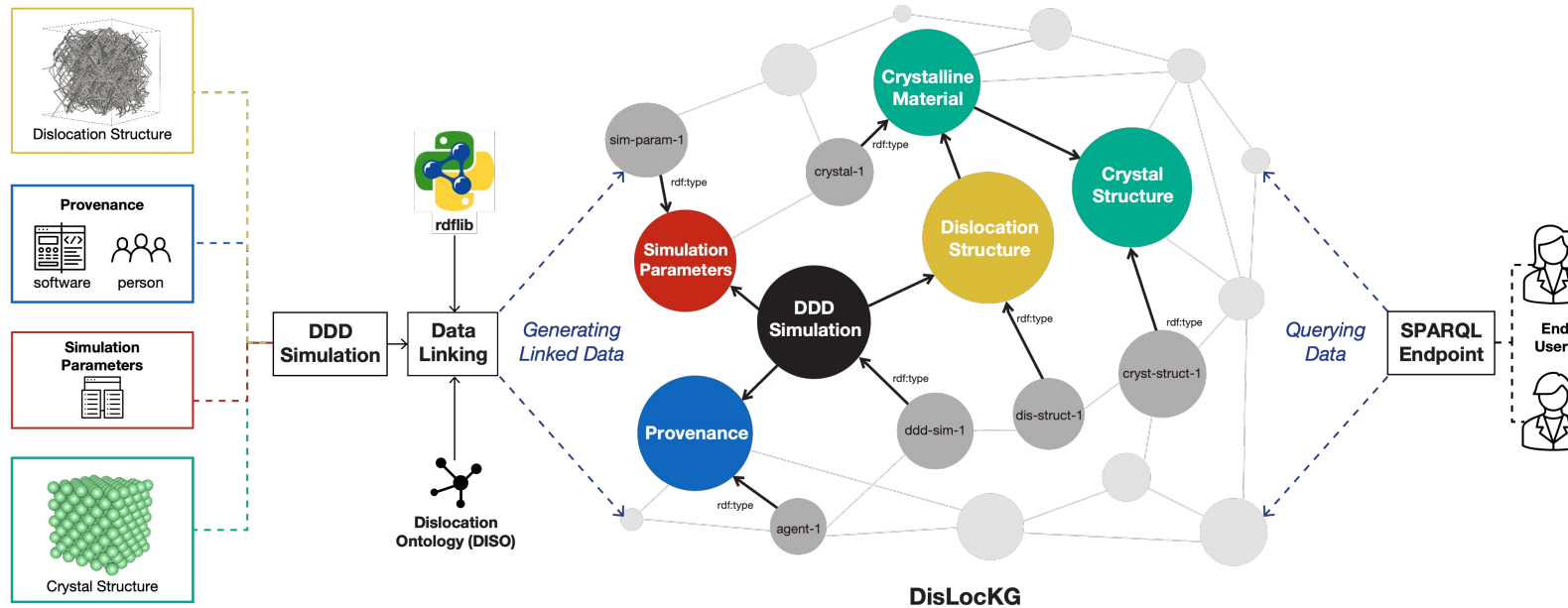
[8] <https://dl.acm.org/doi/abs/10.1145/3555776.3578739>

[9] <http://www.dierk-raabe.com/multiscale-modeling/>

# ONTOLOGY APPLICATIONS

## MODELING DISLOCATION DYNAMICS DATA

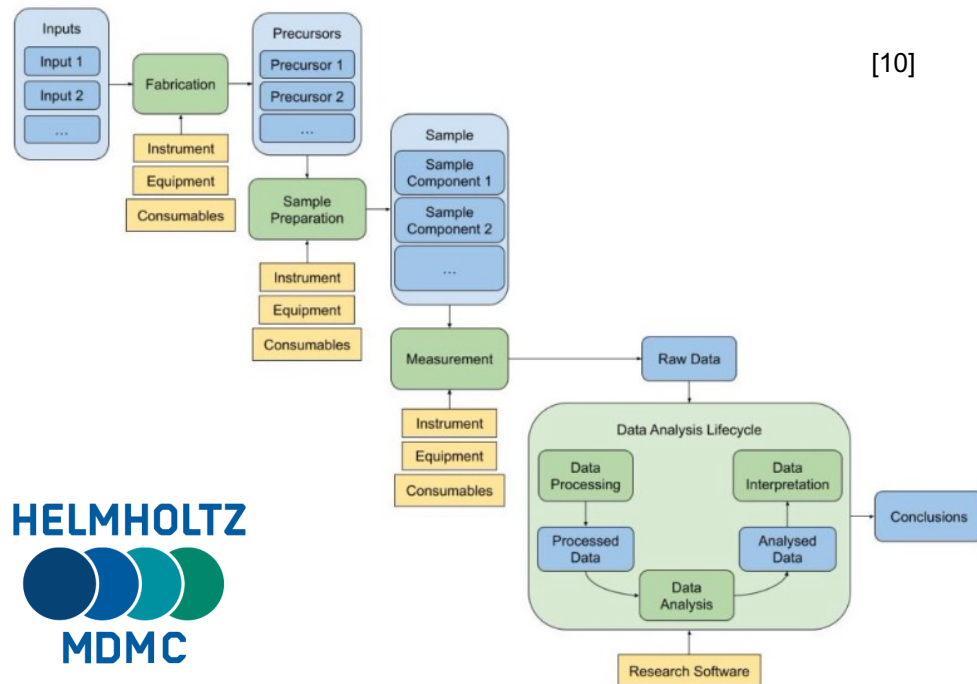
- Dislocation dynamic (DD) simulation
  - We use Dislocation Ontology (DISO) to annotate dislocation dynamics data (data linking)
  - Dislocation dynamics data consists of: structure, crystal structure, simulation parameters, and simulation provenance.
  - We generate dislocation simulation linked data as knowledge graph, **Dislocation Knowledge Graph (DisLockKG)**
  - Via its SPARQL endpoint, one can query dislocation simulation data



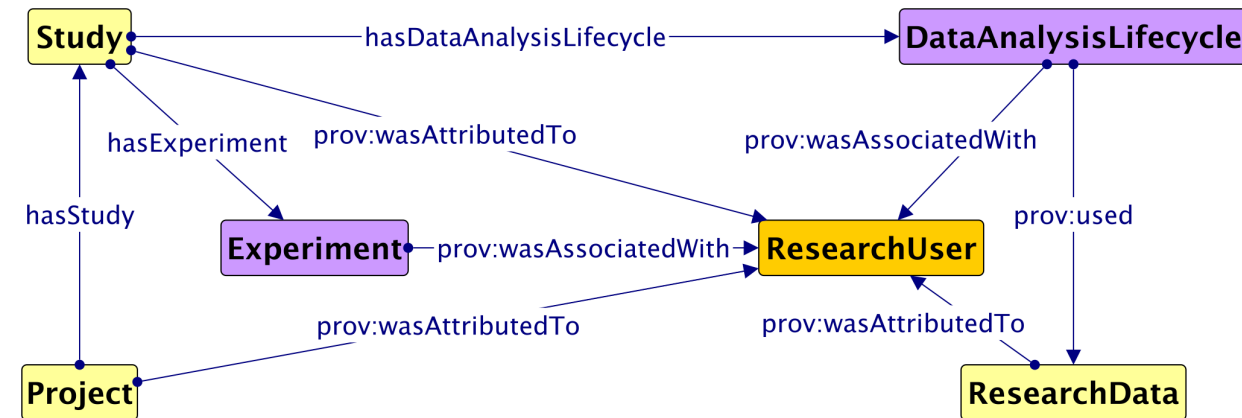
# ONTOLOGY APPLICATIONS

## PROVENANCE ONTOLOGY FOR EXPERIMENTAL WORKFLOW

- The Provenance Information for Materials Science (PRIMA) Ontology:
  - Formalize the experimental workflow into an ontology
  - Used to annotate the experimental data and to increase the reusability by capturing provenance information.



Basic steps experimental workflow



An Excerpt of the PRIMA Ontology  
AZ. Ihsan, M. Jalali, R. Aversa, M. Panighel, E. Osmenaj.



PRIMA

Collaboration through use cases



[10] <https://jl-mdmc-helmholtz.de/mdmc-activities/metadata-working-group/metadata-wg-topics/experimental-workflow/>

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# TAKE-HOME MESSAGE

- Understanding communication involves an encoding (syntax) - decoding (semantics) process.
- Context influences the interpretation of meaning in understanding.
- Formal knowledge representation overcomes the problem of language in knowledge representation.
- Ontology is a kind of formal knowledge representations.

# ACKNOWLEDGEMENTS

