Your name and name of your taxonomy and/or ontology

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- Provisional name of the ontologies: *metal-alloy*, *precipitations-in-metals*

What is the application domain of your taxonomy and/or ontology?

- A pack of compatible ontologies for supporting of workflow during
  - defining of material structure and processes during metal forming and treatment
  - defining models and numerical simulations
  - autonomous adaptation the configuration of continuum materials models

What is the intended purpose of the taxonomy and/or ontology

- Defining items describing polycrystaline materials
- Sharing of a description of physics based models (PBM) and data based models (DBM)
- Matchmaking between materials and PBM or DBM
- Searchable database of PBMs and DBMs – searching possibilities of building a chain of models to solve particular problem
- Validation of an expert system governing choosing PBMs or DBMs for solving particular technological problems
- Supporting knowledge acquisition for an expert system (e.g. generating of decision tables' schemas)

How do you represent the world:

- Currently as a continuum
- Discrete particles will be used in future for mesoscopic models

What are the concepts, with definitions, in the upper level of your taxonomy and/or ontology?

- *Alloy* – named metal alloy (not a particular piece of metal). Described with normative composition (allowable boundaries). Consists of *grains*.
- *Grain* – potentially existing in a particular alloy. Characterized by “*phase*”, consist of crystal lattice with atoms and voids. May also consist of *subgrains* or other *grains*.
- *Multiscale-model* is-a *model* defined in *emmo-models*
- *Multiscale-model* has-components, being ones of *mathematical_models* defined in *emmo-models*

What are the industrial use cases (e.g. in ontology-driven tools) demonstrating the value of the taxonomy and/or ontology?

- The ontologies are developed to support autonomous adaptation of a structure of a multiscale model. Currently it is applied in modelling of heat treatment of A6082 aluminum alloy (academic research).
- Adapive Multiscale Modeling Methodology is aimed at developing of a framework, allowing run-time switching between different configurations of models chain, depending on current state of the models. More details in:
  - Macioł, P., Szeliga, D. & Sztangret, Ł. Int J Mater Form (2018) 11: 867. https://doi.org/10.1007/s12289-017-1396-x
  - Macioł P., Rule-based controlling of a multiscale model of precipitation kinetics, Computer Methods in Material Science, 2019 (in press)
- Current benefits:
  - Adaptive multiscale models involves relatively large number of models. Agreement on numerical level, as well as shared understanding of phenomena is necessary. Ontology is a common reference point
  - The choice of the best configuration of a multiscale model is done with a support of Knowledge Based System (requires rules). Generation of rules is supported by ontology -> relations between ontology entities suggest relations in rules.
- Future benefits:
  - Interoperability of adaptive multiscale framework with marketplaces and BDSSs

What overlaps do you see with other taxonomy and/or ontologies?

- The ontologies are expected to be fully compatible with EMMO set. Hence, any other ontologies were not evaluated from the point of view of compatibility/overlapping
- MatOnto is a potential overlap, however its current state is not clear

What are the (main) relations in your ontology?

- Representation of material from the point of view of material scientists
  - hierarchical has_direct_part relations between entities (alloy, grains, subgrains etc)
  - Grains represents phases (e.g. perlite, cementite etc.)
- Relation of models and material
  - Models can provide properties for materials

What is the knowledge your specific ontology represents?

- Knowledge necessary for a pragmatic description of current practices
- Explanation of the world according to one of the philosophical views called realism/~~conceptualism/nominalism~~

How does your ontology represent the relations between different granularity views on the same object?

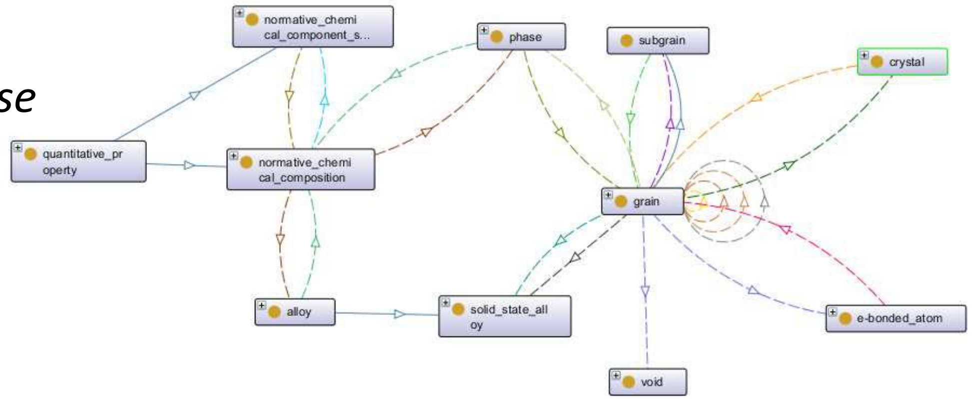
- Within the material branch – granularity in the sense of hierarchical composition
  - An “*alloy*” (potential product made with an alloy) has_direct_proper_parts *grains.*
  - Grain again has_direct_proper_parts *grains* or has_direct_proper_parts *atoms*
  - It is discussed, should all grains of the same phase (e.g. austenite grains in steel) should be treated as a *set*
- Within modelling branch – granularity in the sense of modelled entity
  - Currently all model are continuum.
  - Mesoscopic or atomic models are possible -> material *property* will be evaluated with a model with a particular granularity

How does your ontology represent materials? (point of view of modelling)

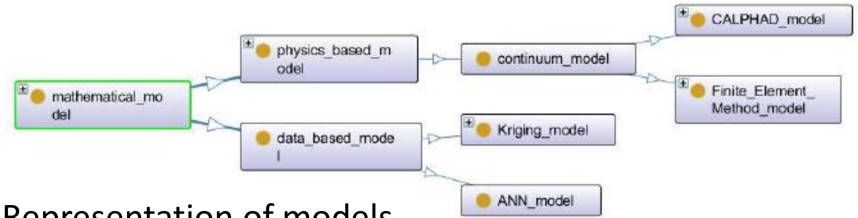
- Currently all models are continuum models

How does your ontology represent materials? (point of view of material science)

- The core component is a *grain (bead)*, being a *direct_proper_part* (in mereological sense) of a *solid-state-alloy*
- A *grain* consist of *subgrains* (if low-angle boundary exists) or "included" *grains* (if included *grain* is other *phase* – precipitation on smaller scale *phase*), both are *direct_proper_part*
- *Subgrain* is-a *grain*
- "Perfect" *grains* (crystal structure) consist of *e-bonded atoms* and *voids*
- There are several relations available (*has_grain_grain*, *has_grain_subgrain* etc., all being child relations of *has_proper_part*)



Representation of material



Representation of models

What type of processes do you address? How does your ontology represent these processes?

- Currently processes are not represented (it is under development)
- It is expected that material processes (e.g. deformation hardening) will be represented from the point of view of physical/chemical processes (e.g. dislocations' migration), which can/should be modelled by particular numerical models.
- Processes are 4D -> history of the material is inseparably connected to its current state
- Processes (understood as technological/manufacturing processes) are not planned to be represented. However, it is expected to bind the ontologies with external ontology of manufacturing processes.

How does your ontology represent manufacturing?

- Manufacturing is not represented
- It is expected to bind the ontologies with external ontology of manufacturing processes.

  Before, an ontology for phenomena's representation must be defined (eg. recrystallization, precipitation etc.). Then, models (e.g. CALPHAD_model) will be bound to phenomena (precipitation) and phenomena will be bound to manufacturing process (like "heat treatment" or "aging")

How does your ontology address the circular connection between physical properties, materials models (see definition in RoMM Review of Materials Modelling VI) and measurement?

- In fact, all represented items are abstractions. Engineering materials are imperfect, hence there is no crisp properties like chemical composition or tensile strength.
- Measurements include error (measure error, simplification error, material uncertainty etc.)
- Numerical models include error (modelling error, simplification error, material uncertainty etc.)
- There is a distinction between a "nominal" property and measure/computed property
- Currently measurements (experiments) are not represented by ontology. It is expected to relate to external ontology for that. It is expected that multiply measurements will be related to a single alloy (including i.a. measured chemical composition)
- A single model (PE+MR) can be related to one or more alloys. For a single model, one or more sets of MR coefficients might be related to a single alloy. In other words, many models differing (slightly) only with coefficients might be valid for a single alloy.

What is the representation language and implementation (logics)?

- OWL-DL
- Consistent with EMMO

- **I herewith confirm that you can publish the attached slides at the EMMC website.**