Geophysical Research Abstracts
Vol. 18, EGU2016-10241, 2016
EGU General Assembly 2016

Semantic modeling of the structural and process entities during plastic deformation of crystals and rocks

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We are semantically modeling the structural and dynamic process components of the plastic deformation of minerals and rocks in the Plastic Deformation Ontology (PDO). Applying the Ontology of Physics in Biology, the PDO classifies the spatial entities that participate in the diverse processes of plastic deformation into the Physical_Plastic_Deformation_Entity and Nonphysical_Plastic_Deformation_Entity classes. The Material_Physical_Plastic_Deformation_Entity class includes things such as microstructures, lattice defects, atoms, liquid, and grain boundaries, and the Immaterial_Physical_Plastic_Deformation_Entity class includes vacancies in crystals and voids along mineral grain boundaries. The objects under the many subclasses of these classes (e.g., crystal, lattice defect, layering) have spatial parts that are related to each other through taxonomic (e.g., Line_Defect isA Lattice_Defect), structural (mereological, e.g., Twin_Plane partOf Twin), spatial-topological (e.g., Vacancy adjacentTo Atom, Fluid locatedAlong Grain_Boundary), and domain specific (e.g., displaces, Fluid crystallizes Dissolved_Ion, Void existsAlong Grain_Boundary) relationships.

The dynamic aspect of the plastic deformation is modeled under the dynamical Process_Entity class that subsumes classes such as Recrystallization and Pressure_Solution that define the flow of energy amongst the physical entities. The values of the dynamical state properties of the physical entities (e.g., Chemical_Potential, Temperature, Particle_Velocity) change while they take part in the deformational processes such as Diffusion and Dislocation_Glide. The process entities have temporal parts (phases) that are related to each other through temporal relations such as precedes, isSubprocessOf, and overlaps.

The properties of the physical entities, defined under the Physical_Property class, change as they participate in the plastic deformational processes. The properties are categorized into dynamical, constitutive, spatial, temporal, statistical, and thermodynamical. The dynamical properties, categorized under the Dynamical_Rate_Property and Dynamical_State_Property classes, subsume different classes of properties (e.g., Fluid_Flow_Rate, Temperature, Chemical_Potential, Displacement, Electrical_Charge) based on the physical domain (e.g., fluid, heat, chemical, solid, electrical). The properties are related to the objects under the Physical_Entity class through diverse object type (e.g., physicalPropertyOf) and data type (e.g., Fluid_Pressure unit 'MPa') properties. The changes of the dynamical properties of the physical entities, described by the empirical laws (equations) modeled by experimental structural geologists, are modeled through the Physical_Property_Dependency class that subsumes the more specialized constitutive, kinetic, and thermodynamic expressions of the relationships among the dynamic properties. Annotation based on the PDO will make it possible to integrate and reuse experimental plastic deformation data, knowledge, and simulation models, and conduct semantic-based search of the source data originating from different rock testing laboratories.