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Reproducible workflows for the generation of material parameters for multiphysics simulations from experiments.

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Abstract

The applicability of computational model depends critically on the availability of parameters for the material at hand. This hold in particular for multiphysics models at the microstructure scale. These models, in contrast to e.g. molecular dynamic models, require the explicit integration of all considered mechanism, such as evolution of dislocation densities, heat generation due to plastic dissipation, influence of chemical composition on dislocation velocities to name but a few. Following the "Batteries Included Philosophy" of the Python programming language, the team of DAMASK®, the Düsseldorf Advanced Material Simulation Kit aims to include a large and curated dataset of configuration files. In this presentation we will show on several examples how various experiments - nano-indentation, tensile tests, XRD-based texture measurements, and lattice strain measurements can be used to obtain parameters for crystal plasticity and multiphysics models. It is also discussed how automated workflows contribute to the generation of FAIR (findability, accessibility, interoperability, and reusability) datasets.

Keywords:

crystal plasticity micromechanics FAIR data