

Machine Learning based Multiscale Modeling of Deformation of Multiphase Microstructures

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For understanding process-structure-property relations, application of artificial intelligence (AI) is becoming increasingly important. Machine learning (ML) architectures have already demonstrated exceptional success in the fields of object detection, pattern recognition, image segmentation, image restoration etc. In the recent past, ML models are being explored aggressively in the area of integrated computational materials engineering (ICME) and material genome initiative (MGI). By using ML and data science, reduced order models can be developed for design of next generation materials and process optimizations. Such models are inherently capable of linking various multiscale features present in the microstructure to pre-specified properties. These models are highly predictive and have high throughput. The overall prediction time is shorter by orders of magnitude as compared to classical numerical methods e.g. finite element modeling. The challenge in development of ML based models is that these models require an enormous amount of training data. For fulfilling this requirement, physics based models e.g. crystal plasticity (CP) models are used for generating surrogate data.

Experimental investigation of multiscale plastic deformation of multiphase microstructure is very time consuming and effort taking. Although, mechanical test data can be complemented with many techniques including electron back scattered diffraction (EBSD) data, overall exercise is expensive, effort taking and more prone to human error. Crystal plasticity finite element method (CPFEM) based simulations have been traditionally used for analysis of plastic deformation of metals. However, CPFEM simulations are computationally expensive for complex boundary conditions. In this work we propose a model / set of machine learning based models that are able to predict macroscopic properties based on microscopic features.

Keywords: Machine Learning, Multi-Scale, Multi-Physics, Crystal Plasticity