Data-driven and Physics-informed Numerical Methods for Assessing Mechanical Properties of Polycrystalline Materials

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Abstract

We propose two neural network pipelines for substituting micromechanical computations on regular grids with periodic boundary conditions, usually tackled by spectral approaches. Synthetic polycrystalline microstructures are generated according to a stochastic 3D model [1], while ground-truth data for validation is provided by an FFT solver. The first surrogate model [2] deals with the modeling of linear elasticity by a physics-informed approach, where learnable modules are coupled to nonlearnable layers in order to fulfill certain physical conditions by construction. We demonstrate that the pipeline is able to train without any ground truth from standard solvers, in a self-supervised scheme. After training, our predictor is able to accurately link a microstructure's crystal orientation field to its corresponding solution field for a given imposed macroscopic strain. We show how the model could be further exploited to solve certain inverse problems. The second surrogate model deals with predicting the toughness value of a polycrystalline stochastic volume element assessed via phase-field FFT computations. We show that a neural network trained with double supervision is able to surpass a singly-supervised one. Finally, significant speedups are provided by the trained neural network, able to predict not only the toughness of an unseen microstructure, but also the continuous damage field associated to it, providing physical explainability.

References

1. P. Rieder, M. Neumann, L. Monteiro Fernandes, A. Mulard, H. Proudhon, F. Willot, V. Schmidt. Stochastic 3D microstructure modeling of twinned polycrystals for investigating the mechanical behavior of γ-TiAl intermetallics, *Computational Materials Science* **238**, 112922, 2024.

2. L. Monteiro Fernandes, S. Blusseau, P. Rieder, M. Neumann, V. Schmidt, H. Proudhon, F. Willot. A physics-informed 3D surrogate model for elastic fields in polycrystals, *Computer Methods in Applied Mechanics and Engineering* **441**, 117944, 2025.