Prediction of the plastic response of polycrystalline materials subjected to a periodic boundary condition using Material Knowledge Systems.

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Abstract:

The polycrystalline nature of metals employed in advanced technological applications causes for their plastic response to be controlled by its distribution of crystallographic orientations, also known as texture. Current computational frameworks are capable of procuring accurate predictions of the anisotropic plastic response of these complex material systems by integrating variational approaches (in the form of finite element methods) into the kinematical theory of the deformation of polycrystalline materials. However, these approaches, also referred as Crystal Plasticity Finite Element (CPFE) approaches, require significant computational resources because they iteratively solve highly non-linear, numerically stiff crystal plasticity constitutive equations. Additionally, these approaches are not capable of leveraging previously obtained predictions since a computationally intensive numerical simulation has to be performed to procure the response of a metal with a new/modified texture. This work presents a data-driven reduced-order model capable of accurately predicting the plastic response of any FCC material in a computationally efficient manner for an imposed periodic boundary condition. This reduced-order model was built using the Material Knowledge System localization framework and leverages the results of a pool of previously performed CPFE simulations to accurately predict the plastic response of any new FCC material in a computationally inexpensive fashion.