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A Mechanics-Informed Deep Learning Constitutive Model for Predicting Strain-Rate-Dependent Microstructural Evolution

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ABSTRACT

Surface severe plastic deformation (S^2PD) processes can generate pronounced near-surface microstructural gradients, high defect densities, and strong strain-rate-dependent mechanical responses. Predictive modeling of the coupled evolution of stress and microstructure is therefore essential for understanding process–structure–property relationships and for supporting constitutive development for engineering applications. In this work, we present a mechanics-informed deep learning constitutive model (MIDLCM) for sequential prediction of macroscopic stress response together with key microstructural descriptors, namely dislocation density and twin volume fraction. The framework combines recurrent neural-network-based history encoding with attention-enhanced temporal feature interaction and mechanics-informed elastoplastic constraints, enabling history-dependent constitutive prediction with improved physical consistency [1,2].

The model is trained using data generated from a calibrated polycrystalline crystal-plasticity constitutive framework [3-5], with experimental guidance from the strain-rate-dependent tensile behavior of a CrFeNi medium-entropy alloy [6]. The current study focuses on constitutive prediction across a wide strain-rate range from quasi-static to dynamic conditions and evaluates the model under representative uniaxial and proportional biaxial loading paths. Results show that MIDLCM accurately captures strain-rate-dependent stress–strain behavior and the associated evolution of dislocation density and twinning activity. In particular, the model reproduces the distinct dislocation accumulation regimes and the transition from dislocation-dominated to twinning-assisted plasticity as the strain rate increases.

Rather than serving as a complete finite-element framework at this stage, the present model is intended as a constitutive-level kernel for efficient microstructure–mechanics coupled prediction. Its current validation is focused on material-point constitutive responses under representative loading conditions, while extension to more complex non-proportional loading histories and finite-element implementation remains a future direction. The proposed approach provides a physically interpretable and computationally efficient surrogate for conventional polycrystalline crystal-plasticity simulations and offers a useful basis for future integration into finite-element analysis of S^2PD and related surface engineering processes.

KEYWORDS

Constitutive modeling; strain-rate dependence; microstructural evolution; dislocation density; twinning; crystal plasticity; deep learning

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