

Fast Assessment of Metal Performances Through Dislocation Physics and Machine Learning



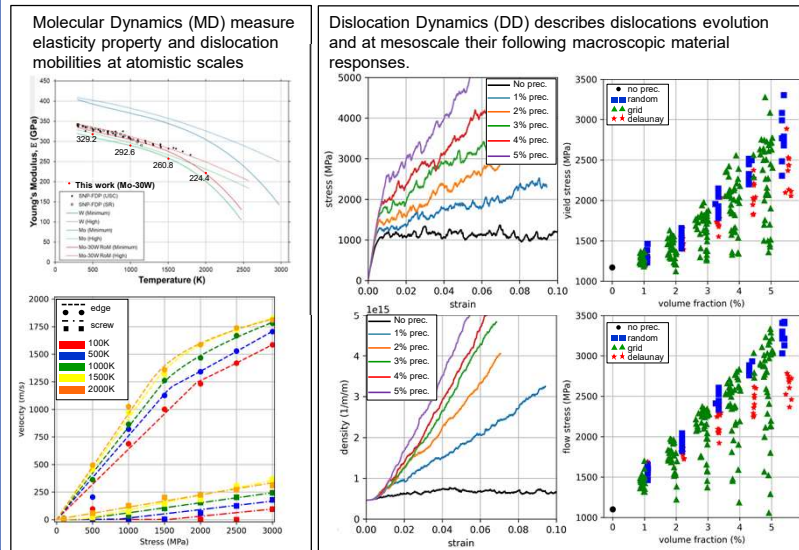
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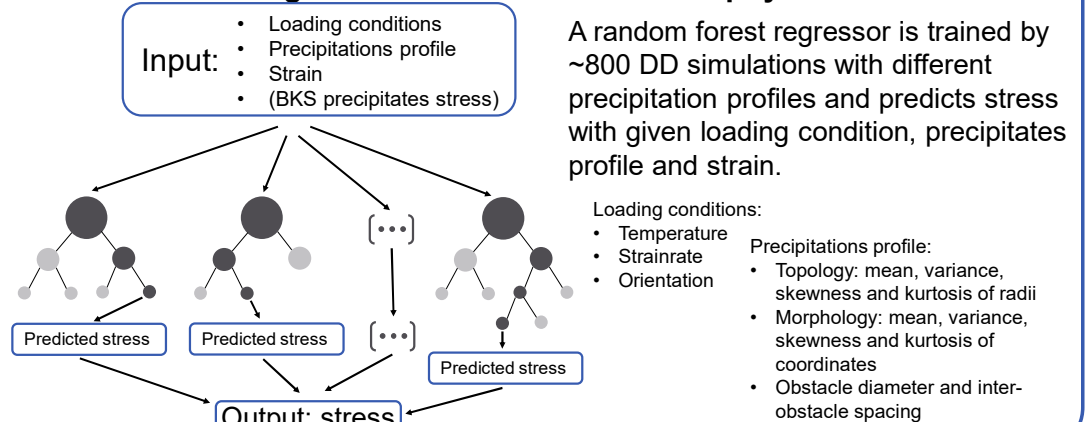
1. Abstract

The microstructure of metals is key to their mechanical properties. The types, density, composition and morphology of crystal defects all have pronounced impact on the properties. Changes to the microstructure occurring during processing and use can be very striking. The emerging technology additive manufacturing (AM) has the potential to improve performance by allowing optimized designs, but the process and environments can lead to unusual microscale features whose properties must be understood and characterized to enable higher technological readiness levels and application. Experimentally, an extensive evaluation of mechanical properties of 3D printed metals is a challenge, and anomalous effects related to the AM process add complexity. We present a new machine learning (ML) model predicting mechanical response based on dislocation mediated plasticity simulations. A large set of 3D discrete dislocation dynamics simulations with wide ranges of loading conditions is transformed to preprocessed data ready for training with the ML model. The trained model can predict the mechanical response of Mo30W for a given microstructure evolution, providing key information essential for optimization of AM processing.

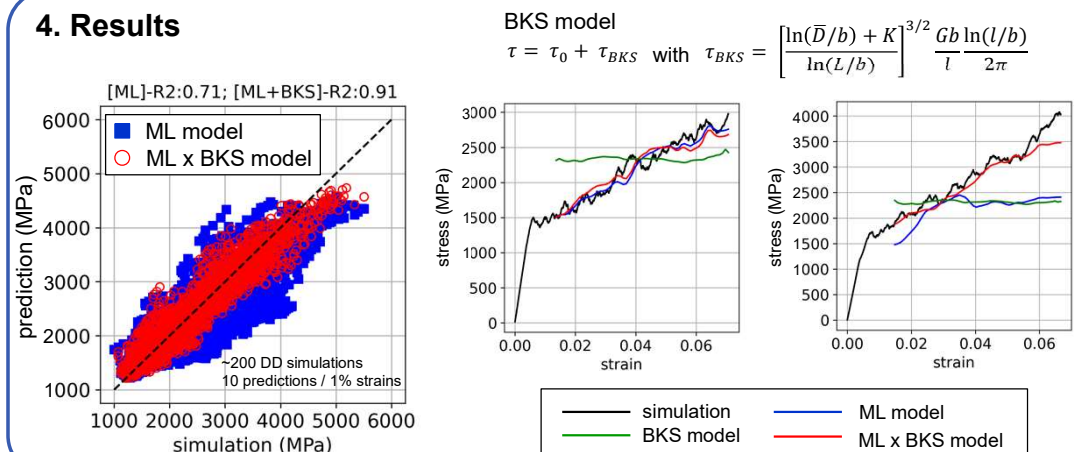
2. Multiscale modeling of Mo30W plasticity



3. Machine learning model based on dislocation-physics simulations



4. Results



5. Engagement and Forward Work

- Effects of grain and grain boundary structures are currently being added in the ML model
- The current work will be used as a key in optimization of AM processing parameter