

MATERIALS ENGINEERING SEMINAR

“Computational Modeling of Dislocation Microstructure Patterns at Small Strains Using Continuum Dislocation Dynamics”

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ABSTRACT

Self-organized dislocation structures in deforming metals have a strong influence on the mechanical response of metals. However, accurate prediction of these patterns remains a challenge due to the complex dynamic and multiscale nature of the underlying process. This dissertation focuses on the development of a theoretical framework for continuum dislocation dynamics (CDD) models to predict dislocation microstructure formation at small strains, along with corresponding numerical simulation results. CDD models have the capability to incorporate plasticity physics spanning different time and length scales while capturing the dislocation motion explicitly within reasonable computational time. A typical model consists of two components: crystal mechanics, formulated as an eigenstrain problem, and dislocation dynamics, treated as a transport-reaction problem. In the first part of the thesis, a novel framework is introduced to solve the dislocation transport by decoupling the system of transport-reaction equations and enforcing the dislocation continuity constraint on individual slip systems. The results obtained from this framework demonstrate high accuracy and computational efficiency, significantly enhancing the predictive capabilities of the model. Building upon the framework, a statistical analysis of stress fluctuations in discrete dislocation dynamics (DDD) simulations is conducted to understand the relationship between coarse-grained average stress and local stress states. This analysis is motivated by the need to accurately capture dislocation reactions, such as cross-slip, which strongly depend on the local stress state, using the coarse-grained approach in CDD. The results revealed that the difference between the local and the coarse-grained states can be characterized using a Cauchy distribution. Consequently, a novel strategy is proposed to incorporate these statistical characteristics into the CDD model, yielding cross-slip rate predictions that align well with DDD results. In the final part of the study, the developed framework is applied to investigate the dislocation pattern formation during the early stages of cyclic loading. The simulation results successfully capture the formation of dislocation vein like structure and provide insights regarding the formation of labyrinth structure observed in experiments during cyclic loading at saturated state.

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Place: ARMS 1021 or via Zoom: <https://purdue-edu.zoom.us/j/5211402390>