Microstructural entropy and stored energy in modeling recrystallization and microstructure-property relationships in polycrystals.

While empirical laws like Hall-Petch have long been known to give inverse relationship between average grain size and polycrystalline material strength, complete understanding of the role microstructure geometry and topology play in coarsening and mechanical deformations is still missing. This talk compares different types of entropy measures that may be used to characterize microstructure disorder based on their ability to capture deviations in certain mechanical and kinetic properties estimated via large scale numerical simulations. GPU-based simulations of recrystallization based on the stored energy formalism are also discussed. (Received September 16, 2019)