Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A3]Symposium A-3

Chair: Katsuyo Thornton(University of Michigan, Ann Arbor, United States of America) 2018年10月30日(火) $09:45 \sim 11:00$ Room6

[SY-A3]From discrete to continuum dislocations and back: a two dimensional study of microstructure and interaction energies.

OHengxu Song, Stefan Sandfeld (TU Bergakademie Freiberg, Germany)

Continuum dislocation dynamics models, which are proposed to conquer the restrictions of high computational cost that discrete dislocation dynamics models generally experience, have made great progress in the past decades. However, it is inevitable that certain dislocation microstructure information is 'lost' during the averaging/coarse graining process ('upscaling'), for example, dislocation short range interactions. This information, however, is crucial for a correct prediction of the structure-property relation in continuum simulations. We will show a new type of multiscale analysis which is based on the energy density of 2D systems, where we identify the 'missing' information during coarse graining for arbitrary averaging resolution. This methodology can be directly generalized to 3D systems of curved dislocations. Furthermore, based on our database, we will be able to benchmark a number of existing 2D continuum formulations for dislocation interaction. Last but not least, we will show that our data base also will be a useful starting point for recovering statistical information of (ensembles of) discrete dislocations from continuum field data during 'downscaling'.