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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 ~ 11:00 Room6

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### [SY-A3] Plasticity and microstructure evolutions at the mesoscale: towards and integrated framework.

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A Fast Fourier Transform (FFT) based hybrid discrete dislocation dynamics (DDD) and cluster dynamics (CD) tool is introduced to study plasticity and microstructure evolution in polycrystalline media. The overall intent of the work is to introduce a unified modeling platform applicable at the tens of micron scale that allows for the validation and calibration of constitutive models and rate theory models used at higher length scales. In addition, the proposed framework aims at leveraging novel/advanced characterization methods. As such the model will be able to be directly compared against in-situ characterization methods (TEM, X-Ray diffraction). With regards to the modeling framework, in addition to its common treatment of plasticity, DDD in combination with FFT methods allows for the description of dislocations both as discrete and as continuous objects, thereby providing an ideal linkage with higher order constitutive modeling, which will be demonstrated by taking the example of grain boundary/dislocation interactions and in bicrystals and polycrystals. Further, an application of this framework to the case of twin propagation in hcp metals will be shown. Finally, the coupling between DDD and CD provides for a treatment of the role of dislocation microstructures on the evolution of radiation-induced damage as well as for the quantification of plasticity induced by irradiation. This will be illustrated in the case of pure body centered cubic Iron in which a mapping of the dominant deformation processes as a function of temperature, stress and irradiation condition will be presented.