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)
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[SY-A3]Advances in microstructure prediction: a FFT-based Dislocation Dynamics approach

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Discrete Dislocation Dynamics (DD) is a well-established simulation technique aimed at reproducing the collective behavior of dislocations at the mesoscale. Despite the considerable progresses made in last decades, DD simulations are still unable to precisely reproduce the microstructure of large poly-crystals and, especially, of irradiated polycrystalline materials. An important step in the development of predictive simulations of this class of materials is the improvement of the numerical capabilities of DD codes to model dislocation properties in large volumes representative of the materials microstructures.
Here we propose a promising strategy based on the coupling between two advanced simulation tools. First, the Discrete-Continuous Model (DCM) is employed [O. Jamond et al., Int. J. Plast. 80,19(2016)]. This numerical model based on the Eigenstrain theory, couples an extensive DD simulation code (microMegas), to an elastic solver dedicated to boundary value problems resolution. The DCM allows for the rigorous solution of dislocation-surface and -interfaces interactions and has been proven to efficiently model plasticity in nano- and micro-objects. Nevertheless, its application has been limited to samples of few mm in size. Second, to overcome this difficulty, we employ a solver based on Fast Fourier Transform (FFT) calculation [Bertin et al. Modelling Simul. Mater. Sci. Eng. 23,065009 (2015)]. In particular, we employ AMITEX_FFTP, a new distributed parallel elastic solver based on FFT calculation. Using this approach, the stress state definition in the simulated volumes can be increased from a 64x64x64 grid to a 1024x1024x1024 one, hence allowing the simulation of realistic dislocation density in a multi-grains periodic volume over significant plastic strains (5-10%). In summary, we aim at improving mechanical properties predictions by taking into account both the complexity of multi-crystalline materials microstructure and the local properties of dislocations.