Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A4] Symposium A-4

Chair: David L McDowell(Woodruff School of Mechanical Engineering, Georgia Institute of Technology, United States of America)

2018年10月30日(火) 11:15 ~ 12:30 Room6

[SY-A4]Effective Transport Properties of Polycrystalline Materials

Invited

William Beck Andrews[1], Min-Ju Choe[1], Erik Hanson[1], Max Powers[1], Hui-Chia Yu[1,2], ○Katsuyo Thornton[1]

(1.University of Michigan, Ann Arbor , United States of America, 2.Michigan State University , United States of America)

Most solid materials have surfaces, interfaces, and grain boundaries that enhance or hinder transport; as a result, the properties of polycrystalline solids can be vastly different from their intrinsic properties, especially in nanocrystalline materials. Diffusion in polycrystalline materials plays an important role in a wide range of material systems, including those found in batteries and solid oxide fuel cells. Due to the computational expense in explicitly considering the grain boundary network, establishing rational design rules for nanocrystalline materials with desired transport properties remains a challenge. We apply the Smoothed Boundary Method to evaluate the effective diffusivity of polycrystalline materials with a range of grain morphologies. We find that the anisotropy of grain morphologies plays a critical role in the overall transport behavior, which cannot be quantified using the classical mean field theories. The results are used to obtain an expression for mixed-pathway transport that is capable of universally predicting the effective diffusivity in complex polycrystalline solids without the use of computationally intensive simulations. Such an approach enables efficient simulation of transport in larger-scale systems while accurately capturing the effects of grain morphologies.