

Summer Collaborators Report

Weiqing Ren

Our research group consisted of Weiqing Ren (NUS, Singapore), Yang Xiang (HKUST, Hong Kong) and his student Luchan Zhang. We visited IAS in the period of 7-31 July 2017. During our visit, we focused on the theory and numerical methods for modeling thermally-activated transition (rare) events, and their application to grain boundary motions in crystalline solids.

Grain boundary migration plays critical role in the properties of crystalline materials. At the atomistic scale, the grain boundary motion involves complex mechanisms with different energy barriers. These mechanisms and energy barriers determine the mobility of the grain boundary, which is one of the key object in modeling grain boundary motions. The computation of the mechanisms (e.g. transition pathways) and the energy barriers associated with the grain boundary motion is a challenging task at the atomistic scale, due to the large number of degrees of free freedom of the configuration space and the exponentially-long time scale associated with the barrier-crossing events. To overcome these difficulties, we discussed the possibility of studying this problem in a coarse-grained space consisting of a set of collective variables. The collective variables are chosen as the averaged quantities that characterize the local crystal structures. The transition pathway (i.e. the mean free energy path) and the free energy barriers in this coarse-grained space can then be computed using the string method, an efficient technique originally developed by Ren et al. for modeling rare events in complex systems. The mean force, which drives the evolution of the string in the collective variable space, can be computed on-the-fly using constrained molecular dynamics. In the future, we will implement these ideas in the study of grain boundary motions in various types of crystalline solids.

We had a fruitful collaboration and have made significant advances in our joint research project during our visit of IAS. We appreciate the opportunity and the excellent research environment IAS has provided to us.