東京大学大学院工学系研究科　総合研究機構

結晶界面工学研究室

Crystal Interface Laboratory, The University of Tokyo

Crystal Interface Lab. Seminar Series

# “Atomistic modelling of dislocations and interfaces in metals and oxides”


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The optimal performance of advanced materials requires an impeccable understanding of the microstructural defects that control mechanical and functional properties. Modelling these defects directly from the atomic scale has made tremendous progress, in particular with the dissemination of first-principles calculations that can yield quantitative predictions. Such calculations remain however limited in space and time and more approximate potentials are still needed and undergo currently a revolution with the development of machine learning potentials.

In this seminar, I will present recent works that lead to a new understanding of dislocations and phase boundaries in metals and ceramics, highlighting the successes and limitations of first-principles calculations and interatomic potentials. Topics to be covered will include dislocation core reconstructions in BCC metals due to interstitial solutes, twin boundary mobility in HCP metals as well as transformation-induced plasticity in zirconia-based ceramics.

Main meeting room at Institute of Engineering Innovation

工学部総合研究機構９号館１階　大会議室

2022, April 20th (Wed.)　10:00～11:30