UNIVERSITY OF CALIFORNIA, IRVINE

THE DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING

Is Proud to Host a Seminar by:

STAFF SCIENTIST TIMOFEY FROLOV

Thermodynamics and Computational Modeling of Materials

Lawrence Livermore National Laboratory

Thursday, October 27, 2022

2:00-3:20 PM

Location: McDonnell Douglas Engineering Auditorium

ATOMISTIC SIMULATIONS OF GRAINS BOUNDARY STRUCTURE AND BEHAVIOR

Abstract: Grain boundaries greatly influence many properties of engineering materials. Accurate prediction of their structure and possible transitions using atomistic modeling are important for strategies that aim to improve properties of materials. Recent years have seen a rapid growth of evidence suggesting that materials interfaces are capable of first-order structural transformations in which the interface properties undergo discontinuous changes. Experiments have linked these transitions to abnormal grain growth in ceramics, activated sintering and liquid metal embrittlement and raised a number of fundamental questions concerning the atomic structures and kinetic properties of these interface phases. The first part of the talk I will describe the state-of-the-art modeling tools we use to predict grain boundary phases and new methodologies to model grain boundary phase transformations in metallic systems.

In the second part of the talk, I will focus on our recent massively parallel atomistic simulations of bicrystal deformation performed on scale approaching microns using the cross-scale method. The scale of these simulations allows to model dynamic evolution of dislocation networks in the presence of grain boundaries with atomic resolution to reveal new details about the nature of their interaction. *This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.*

Bio: Timofey Frolov is a staff scientist at Lawrence Livermore National Laboratory, his research expertise is in thermodynamics and computational modeling of materials. He uses state-of–the-art computational tools to model materials interfaces and interface related phenomena and investigate their impact on materials properties. He received his PhD from George Mason University in 2012 where he worked on developing a thermodynamic theory of solid-solid and solid-liquid interfaces that included effects of non-hydrostatic stresses. After the PhD, he did a postdoc as a Miller Fellow at UC Berkeley and subsequently a postdoc at Lawrence Livermore National Lab, where he primarily worked on grain boundary phase transitions in metallic systems. He is a recipient of a prestigious Mercator Fellowship from the German Science Foundation. This award funds a collaboration with the microscopy group at Max Plank Institute in Germany to couple his modeling efforts with direct experimental observations of GB transitions in alloys. In 2022 he received DOE Early Career Award to work on tungsten alloys for fusion energy applications.