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CIVIL ENGINEERING

Time: Monday, October 14, 2019 2:00 – 3:00PM
Location: Fluor Daniel (EIB) Room 132

Impact of Molecular Dynamics Simulations on Materials Science

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Molecular dynamics (MD) simulations are playing an increasingly important role in materials science. Here we review some recent case studies performed at Sandia. In the first example, we show how time averaged MD simulations are used to obtain accurate dislocation energies. In the second example, we demonstrate how MD can be used to validate existing thin film misfit dislocation theories. In the third example, we describe our efforts to develop an Fe-Ni-Cr-H interatomic potential to enable studies of hydrogen embrittlement in stainless steels. In the fourth example, we further present our work on developing an Al-Cu-H interatomic potential to enable simulations of hydrogen embrittlement in Au-Cu alloys. Finally, we highlight the significance of MD simulations in many other applications.

Xiaowang_Zhou is a principal member of technical staff at Sandia National Laboratories. He received his Ph.D. from the Department of Mechanical Engineering at Clemson University in 1995 under the guidance of professor Mica Grujicic. Prior to Sandia, Dr. Zhou worked as a research scientist at the University of Virginia for 12 years. His current research work mainly focuses on hydrogen embrittlement in various structural materials (e.g., Fe-C steels, Fe-Ni-Cr stainless steels, Al-Cu alloys), thermodynamics and kinetics of hydrogen storage materials (e.g., Mg-B-H systems), and hydrogen permeation in zirconium alloys.