

Department of Mechanical and Biomedical Engineering

Seminar Series

Computer simulation of irradiation effects in materials

Dr. Shijun Zhao

Postdoctoral Research Associate
Oak Ridge National Laboratory, USA

Date	March 27, 2018 (Tuesday)
Time	3:00 – 4:00pm
Venue	Room B6619 (MBE Conference Room) 6/F, Yeung Kin Man Academic Building

Abstract

As an important option for clean energy, advanced nuclear fission and nuclear fusion energy have received extensive attention nowadays and are under active development. One of the grand challenges in continued utilization of nuclear energy systems is to design radiation-tolerant structural materials. For this purpose, understanding irradiation effects in materials at the electronic and atomic scale is extremely important. By means of *ab initio* calculations based on density functional theory (DFT), molecular dynamics (MD) simulations and kinetic Monte Carlo (KMC) methods, the defect production, formation, migration, and clustering processes in a variety of materials have been investigated. Specifically, this presentation will show computer simulation results about radiation effects in low-dimensional materials (graphene, carbon nanotube), ceramics (SiC, ZrO₂ and MAX phase) and metal alloys (pure Ni and high entropy alloys). Different simulation techniques are concurrently or sequentially employed to shed light on defect dynamics in these materials. The obtained results are compared with experiments and help to reveal radiation damage mechanisms. These results elucidate driving mechanisms for irradiation-induced damages in different materials and contribute to materials design for improved radiation performances. At last, the application of computer simulation in energy storage materials will also be discussed.

About the Speaker

Shijun Zhao is currently a Postdoctoral Research Associate at Oak Ridge National Laboratory. Dr. Zhao earned his bachelor's degree in Physics in 2008 and his Ph.D. in Nuclear Engineering in 2013 from Peking University. His Ph.D. research focuses on radiation effects in ceramics and low-dimensional materials based on *ab initio* methods and molecular dynamics simulations. Before he came to Oak Ridge, Dr. Zhao spent two years at College of Engineering in Peking University, where he worked on excited electron dynamics in materials under high-energy ion or laser irradiation using *ab initio* methods. Dr. Zhao's current research revolves around radiation performance in a novel series of Ni-contained concentrated solid solution alloys. Dr. Zhao has authored or co-authored more than 40 technical papers with more than 680 citations and has contributed to 3 topical reviews in the field of radiation damage in concentrated alloys.

Enquiry: 3442 8420

All are Welcome!