BEN-GURION UNIVERSITY OF THE NEGEV
P.O.B 653, BEER-SHEVA 84105, ISRAEL

אוניברסיטת בן-גוריון בנגב
ת.ד. 653, באר-שבע 84105

DEPARTMENT OF MECHANICAL ENGINEERING

SEMINAR

to be held on Thursday, December 13, 2018, 11:00

in the Seminar Room (#117) of the Mechanical Engineering Building (#55)
at the Campus of the Ben-Gurion University of the Negev

Mechanical Properties of Pristine, Polycrystalline and Defective Graphene

Prof. Ivan I. Oleynik

Department of Physics, University of South Florida, Tampa, FL, USA

Abstract:

Recent indentation experiments on graphene have revealed its exceptional strength, making it an excellent candidate for the design of nano- and micro- electro mechanical systems. Surprisingly, experiments indicate that the polycrystalline graphene grown by chemical vapor deposition is as strong as pristine. Moreover, recent experiments involving nanoindentation of graphene have also demonstrated a counterintuitive increase of Young's modulus with increasing concentration of point defects. To rationalize these observations, theoretical input is required to predict the important mechanical properties, as well as to understand the underlying fundamental physics of mechanical response. In this talk, I describe recent advances in large-scale molecular dynamics simulations of mechanical properties of pristine, polycrystalline and defective graphene under conditions mimicking nanoindentation AFM experiments. Such simulations are enabled by accurate description of interatomic interactions by novel screened environment-dependent bond order potential. The atomically resolved characterization of the stress and strain distributions under indenter are used to understand fundamental mechanisms of graphene strength and failure. The breaking strength, crack initiation and propagation are investigated as a function of the grain boundary structure, grain size distribution, concentration of point defects as well as the position of the indenter in respect to these extended and point defects.

Bio: Ivan I. Oleynik is a faculty member in the Department of Physics, University of South Florida, Tampa, FL, USA. He has authored more than 120 papers in international journals. His research covers simulation of matter at extreme conditions of high pressure, high temperature and high strain rates; computer-aided discovery of new materials with unique electronic, vibrational, thermal, mechanical, optical, transport and superconducting properties; novel high-nitrogen content energetic materials, superhard materials, 2D materials for energy applications; development of interatomic potentials for large-scale simulations of materials. He holds M.S. in Physics from Moscow Institute of Physics and Technology and Ph.D. in Physics from Institute of Chemical Physics of Russian Academy of Sciences.
Ivan I. Oleynik is a Fellow of American Physical Society. He was granted the University of South Florida Outstanding Research Award, the ONR/NRL Summer Faculty Research Fellowship, The Royal Society (UK) Research Fellowship award, and AFOSR/EOARD Window on Science award.