DEPARTMENT OF MECHANICAL & AEROSPACE ENGINEERING
WILLIAM MAXWELL REED SEMINAR SERIES

"Mechanics of defects in layered 2D carbon, hot and cold."

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Abstract:

Materials consisting of layered two-dimensional carbon are important for high temperature applications, as in thermal protection systems, and for low temperature applications, such as in next generation microelectronic materials. Here we consider the formation of defects in graphitic carbon as a high temperature material, and in bilayer graphene as a low temperature material. Defect formation due to oxidation at high temperatures is studied using a multi-lattice atomic scale Kinetic Monte Carlo (KMC) model. Our KMC model is unique in that adsorption and diffusion of oxygen on the carbon surface are modeled directly, allowing defects to form on an initially pristine surface as a result of interactions between surface groups such as lactone-ethers and ether-lactone-ethers. The KMC simulations reveal differences in defect shape, defect density, and etch rates across temperatures ranging from 1300K to 2200K. Separately, we consider formation of rotational defects at low temperatures in bilayer graphene systems using empirical atomistic models and density functional theory. We present a dislocation mechanics model for the moiré pattern formed by regions of commensurability and incommensurability in the twisted bilayer. We explain the detailed in-plane relaxation of the moiré, both in-plane and out-of-plane, and we are finally able to link the displacement fields, predicted using our nonlinear elastic dislocation theory, to the presence of superconductivity in these systems – a distinctly low-temperature phenomenon. Across both high- and low-temperature examples, our results show the link between mechanics and electronic structure through defects in the materials.

Speaker Bio:

Harley T. Johnson is the Founder Professor of Mechanical Science and Engineering in the Grainger College of Engineering at the University of Illinois at Urbana-Champaign. His research group studies the effects of strain and deformation on functional properties of microelectronic and optical materials including silicon, carbon, group III-V materials, and 2D materials. He has authored or co-authored more than 100 archival journal publications. He is the Director and PI of the NSF "DIGI-MAT" NRT Program in Materials and Data Science at Illinois, a training grant that supports approximately 30 PhD students across multiple departments. Dr. Johnson also serves Associate Dean for Research in the Grainger College of Engineering. He is a Fellow of ASME and SES, and has received numerous awards for research, teaching, and leadership. He earned an undergraduate degree from Georgia Tech and graduate degrees from Brown University.

Date: Friday, February 3, 2023
Time: 3:00 PM EST
Place: Whitehall Classroom Building 110
Contact: Dr. Jesse Hoagg

Attendance open to all interested persons

College of Engineering

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