DEPARTMENT OF MECHANICAL ENGINEERING
WILLIAM MAXWELL REED SEMINAR SERIES

"Carbon Oxidation at the Atomic Level: A Computational Study on Oxidative Graphene Etching and Pitting of Graphitic Carbon Surfaces"

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Abstract: One of the great challenges in hypersonic flight is the protection of air- and spacecraft against extreme aerodynamic heating. This is often achieved by carbon-based ablative heat shields, which are designed to gradually burn off and thereby mitigate the extreme heat at the vehicle's surface. This burnoff process is called ablation, and it involves oxidation of the carbon material by the impinging oxygenic gas. Hence, in order to accurately predict the recession of the heat shield resulting from ablation for a safe vehicle design carbon oxidation has to be understood on a fundamental level where the surface reactions occur. Graphene and graphite are the characteristic structural elements of solid carbon surfaces, and they are etched by oxygen on the atomic level to form characteristic nano- to micrometer sized pits that are scattered across the material surface. This pitting phenomenon leads to microstructural changes that determine the macroscopic oxidation behavior of the carbon material. While pitting has been observed experimentally for at least a century, comprehensive computational studies have been heretofore missing. In this talk a computational framework developed to study carbon oxidation at the atomic level is presented. It entails a comprehensive, atomic-scale kinetic mechanism for carbon oxidation consisting of elementary surface reactions with reaction rates derived from first principles. The mechanism is implemented using the Kinetic Monte Carlo (KMC) method in order to simulate oxidative graphene etching to relevant time- and lengthscales (up to seconds and hundreds of nanometers), and in a wide range of conditions (temperatures up to 2000 Kelvin, pressures ranging from vacuum to atmospheric pressure). The numerical results reveal in-depth information about the pitting process, which is crucial for modelling of carbon oxidation on meso- and macroscales.

Bio: Simon Schmitt is a Postdoctoral Research Scholar in the Department of Mechanical Engineering at the University of Kentucky. He received his B.Sc. degree in Mechanical Engineering from the Karlsruhe Institute of Technology (KIT) in Germany in 2016. During his undergraduate studies, he spent a semester as a student research intern at the University of Kentucky with Dr. José Graña-Otero in 2015, working on CFD of potential flows. After a 6 month R&D internship at Porsche AG in Weissach, Germany, he returned to Lexington to pursue his doctoral degree under the supervision of Dr. Graña-Otero, which he completed in December 2020. Afterwards, he joined Dr. Alexandre Martin's group as a Postdoc to further investigate and model surface chemistry on ablative carbon materials.

Date: Friday, Mar. 19th
Time: 3:00PM EST
Place: https://uky.zoom.us/j/92940732923
Contact: Dr. Alexandre Martin 257-4462

Attendance open to all interested persons

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