FIRST PRINCIPLES INVESTIGATION OF OXYGEN DEFICIENT CENTERS IN AMORPHOUS SILICA

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Abstract: Amorphous, or vitreous, silicon dioxide ($\alpha$-SiO$_2$) is an extremely important material used in many technological applications from microelectronics to optical transmission media. Whether from manufacturing, irradiation, or even mechanical deformation, charged point defects are present within $\alpha$-SiO$_2$. Understanding the nature of these defects is critical to predicting the reliability and performance of the devices which utilize $\alpha$-SiO$_2$ as a critical material component. Two common examples of charged defect degradation involving amorphous silica are large threshold voltage shifts in metal-oxide-semiconductor transistors and substantial attenuation in optical fibers. Dielectric charging is also an extremely prominent mode of failure for the RF MEMS devices that are of interest to PRISM. A variety of charged defect centers are believed to correspond to oxygen deficient regions within silica, and little is known about the exact structure of these defects at the atomic level.

This talk will focus on work done over the summer of 2009 in which a significant number of oxygen deficient amorphous silica samples were generated through a combination of first-principles based reactive molecular dynamics and density functional techniques. Structural analysis was performed on these samples and four experimentally known oxygen deficient defect centers which have not previously been predicted from first principles were identified. In addition, an analysis of defect formation energies was performed and results were found to be in agreement with previously reported theoretical and experimental results.

Bio: Nathan began his graduate career at Purdue as a Fredrick N. Andrews Fellow in the fall of last year. His research interests lie in advancing the atomic level understanding of the structure, formation, and migration of defects within oxide and nitride systems and at any interfaces which these materials might be a part of through various computational techniques. He is focused on applying this understanding to better predict the reliability and performance of microelectronic devices. A parallel interest lays in the interaction of these defect centers with qubits to determine the feasibility of various proposed quantum information processing material systems.

Refreshments will be served.
For further information please contact Asst. Prof. Alina Alexeenko, alexeenk@purdue.edu
For information about PRISM visit: http://www.purdue.edu/dp/prism/index.shtml