A computational materials post-doctoral position funded by the U.S. Department of Energy is available starting immediately on the atomistic simulation of the initial stages of metal oxidation. The appointment is initially for one year with possible extension up to 3 years. This position is offered by Professor Alan McGaughey (Mechanical Engineering, Carnegie Mellon University, Pittsburgh, PA) and Professor Judith Yang (Mechanical Engineering and Materials Science, University of Pittsburgh), in collaboration with Professors Susan Sinnott and Simon Phillpot (Materials Science and Engineering, University of Florida, Gainesville).

Surface oxidation processes play critical roles in environmental stability, high temperature corrosion, electrochemistry, functional oxide film growth as well as various energy applications, such as fuel cells and hydrogen storage. The objective of this research program is to develop a mechanistic understanding of nano-oxidation via coordinated theoretical and experimental efforts. The successful applicant will apply and extend nucleation rate theory, typically used to describe thin film growth, to the more complex reaction of oxygen with metallic surfaces—ranging from the arrival of oxygen molecules on a metal surface, diffusion, and the nucleation, growth to coalescence of the metal oxide. The successful applicant will develop a KMC code to simulate the complexities of oxygen interactions with a metal surface in 3-dimensions. These KMC predictions, utilizing input parameters obtained via first principles and molecular will then be directly correlated with in situ transmission electron microscopy (TEM) experiments, for comprehensive knowledge of nano-oxidation. A web site on the present KMC code, called TFOx (thin film oxidation) that simulates 3-dimensional irreversible nucleation and growth can be found at www.tfox.org. A PhD in Mechanical Engineering, Materials Science, or similar field is required as is computational background, especially C++.

This project is at the forefront of materials and surface science, with a comprehensive synergy between the different levels of simulation, including electronic structure, molecular dynamics as well as KMC, and experiments. The Places Rated Almanac named Pittsburgh recently as “America’s Most Livable City”. Both the College of Engineering and Mechanical Engineering Department at Carnegie Mellon University are ranked in the top 10 in the U.S. News and World Report Rankings. The University of Pittsburgh is ranked 37th in the world’s top 100 global universities by Newsweek International, and second in the nation for nanoscale research (Small Times, 6(3) 2006).

To apply for this position, please send a resume with the names and contact information for three references, or to obtain more information, please contact Prof. McGaughey and/or Yang:

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