Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Role of oxygen diffusion at Ni/Cr_2O_3 interface in intergranular oxidation of Ni-Cr alloy[1] BHARAT MEDASANI, MARIA SUSHKO, DANIEL SCHREIBER, KEVIN ROSSO, STEPHEN BRUEMMER, PACIFIC NORTHWEST NATIONAL LAB — Certain Ni-Cr alloys used in nuclear systems experience intergranular oxidation and stress corrosion cracking when exposed to high-temperature water leading to their degradation and unexpected failure. To develop a mechanistic understanding of grain boundary oxidation processes, we proposed a mesoscale metal alloy oxidation model that combines quantum Density Functional Theory (DFT) with mesoscopic Poisson-Nernst-Planck/classical DFT. This framework encompasses the chemical specificity of elementary diffusion processes and mesoscale reactive dynamics, and allows modeling oxidation processes on experimentally relevant length scales from first principles. As a proof of concept, a preliminary model was previously employed that limited oxygen diffusion pathways to those through the oxide phase and did not allow oxygen diffusion in the alloy or across oxide/alloy interfaces. In this work, we expand the model to include oxygen diffusion pathways along Ni/Cr_2O_3 interfaces and demonstrate the increasing importance of such pathways for intergranular oxidation of Ni-Cr alloys with high Cr content.

[1]This work is supported by the U.S. Dept. of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. Simulations are performed using PNNL Institutional Computing facility.

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Date submitted: 04 Nov 2015 Electronic form version 1.4