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Investigating Cu Grain Boundary Oxidation via Density Functional Theory, Reactive Force Fields, and Experiment MATTHEW CURNAN, WISSAM SAIDI, CHRISTOPHER ANDOLINA, JUDITH YANG, University of Pittsburgh, Pittsburgh, PA — The presence of grain boundaries in metals is expected to significantly alter metal oxidation behavior due to O diffusion and segregation towards GBs, leading to distinct preferential Cu oxide nucleation behavior on GBs under different thermodynamic conditions. A comprehensive understanding of which O diffusion and oxide nucleation processes occur under particular thermodynamic conditions and over broad sets of GBs is not available. To resolve relationships between stable structures and O diffusion energetics, we develop a methodology based on a Cu/O reactive force field (RFF) trained with Density Functional Theory (DFT) and experimental data. Using this DFT-RFF approach, we determine the O diffusion activation barriers, segregation energetics, and relative GB energy vs. tilt angle profiles of different Cu-O GB systems as functions of temperature. Given that the relative energetics of different GB tilt angles can be accurately predicted and tuned with temperature, the inclusion of these energetics in Cu/O RFFs can help predict experimentally observed GB angle distributions at particular temperatures. When trained with experimental and DFT energetics and structures, these RFFs can be expanded to study the tuning of GB properties for Cu/O and related doped systems.

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