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Multiscale Investigations of the Early Stage Oxidation on Cu Surfaces QING ZHU, University of Pittsburgh, PENGHAO XIAO, XIN LIAN, SHEN-CHE YANG, GRAME HENKELMAN, University of Texas at Austin, WISSAM SAIDI, JUDITH YANG, University of Pittsburgh, UNIVERSITY OF PITTSBURGH TEAM, UNIVERSITY OF TEXAS AT AUSTIN TEAM — Previous *in situ* TEM experiments have shown that the oxidation of the three low index Cu surfaces (100), (110) and (111) exhibit different oxide nucleation rates, and the resulting oxides have 3-dimensional (3D) island shapes or 2D rafts under different conditions. In order to better understand these results, we have investigated the early stages of Cu oxidation using a multiscale computational approach that employs density functional theory (DFT), reactive force field (ReaxFF), and kinetic Mote Carlo (KMC). With DFT calculation, we have compared O_2 dissociation barriers on Cu (100), (110) and (111) surfaces at high oxygen coverage to evaluate the kinetic barrier of sublayer oxidization. We found that O_2 dissociation barriers on Cu(111) surface are all lower than those on (110) and (100) surfaces. This trend agrees with experimental observations that (111) surface is easier to oxidize. These DFT calculated energy barriers are then incorporated into KMC simulations. The large scale ReaxFF molecular dynamics and KMC simulations detail the oxidation dynamics of the different Cu surfaces, and show the formation of various oxide morphologies that are consistent with experimental observations.

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