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Multiscale Investigations of the Oxidation of Stepped Cu Surfaces[1] QING ZHU, Chemical Engineering, University of Pittsburgh, WISSAM SAIDI, Materials Science, University of Pittsburgh, JUDITH YANG, Chemical Engineering, University of Pittsburgh — Defects on metal surfaces can induce non-canonical oxidation channels that may lead to the formation of novel nanostructures. Cu surfaces have been actively researched in the surface science community due to their wide range of applications in many fields. Recently, in situ TEM experiments showed that the oxidation of stepped surfaces promotes the formation of a flat metal-oxide interface through the Cu adatoms detachment from steps and diffusion across the terraces. In order to better understand these results, and to provide a tight bridge between the experiment and theory, we have investigated the Cu (100) oxidation using a multiscale computational approach that employs density functional theory and reactive force field. Our results demonstrate that the step-edge defects induce markedly different oxidation dynamical behavior compared to the flat surface. Additionally, on the stepped-surfaces, we find that the oxidation of the upper-terrace are more favored than the lower-terrace. We show that is behavior is due to a negative Ehrlich-Schwoebel diffusion barrier for oxygen in the ascending direction. The favoring of the oxidation of the top terrace drives Cu diffusion flux from the upper-terrace to the lower-terrace that explains the recent TEM experiments.

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