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Investigation of atomic oxygen embedment into copper surface by DFT calculation[1] MINYOUNG LEE, ALAN MCGAUGHEY, Carnegie Mellon University, SUSAN SINNOTT, SIMON PHILLPOT, University of Florida, JUDITH YANG, University of Pittsburgh — In the oxidation of a Cu(100) surface, the Cu_2O islands grow both into the substrate and parallel to the surface. To investigate the oxide growth into the copper surface, we analyzed oxygen embedment using DFT calculations. Using the nudged elastic band method, we calculated energy barriers for oxygen embedment for different oxygen coverages and different surface morphologies. As the oxygen coverage increases from 0.25 monolayers (ML) to 1.0 ML, the energy barrier decreases and we find an energetically favorable site between the top and second copper layers at an oxygen coverage of 1.0 ML. The different surface morphologies [$c(2\times2)$, missing-row reconstruction and $c(2\times2)$ with 0.25 ML disordered copper vacancy] have comparable energetics and no energetically favorable site for oxygen embedment is predicted. To find the energetically favorable transition states on the missing-row reconstructed Cu(100) surface, we will investigate oxygen embedding paths with and without point defects on the top copper layer.

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