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Order-disorder phase transition of the Cu(001) surface under equilibrium oxygen pressure H. IDDIR, D.D. FONG, MSD, Argonne National Laboratory, IL 60439, P. ZAPOL, CSED & MSD, Argonne National Laboratory, IL 60439, P.H. FUOSS, MSD, Argonne National Laboratory, IL 60439, L.A. CURTISS, CSED & MSD, Argonne National Laboratory, IL 60439, G.-W. ZHOU, J.A. EASTMAN, MSD, Argonne National Laboratory, IL 60439 — Understanding atomic processes involved in catalyzed reactions is of great importance and can be achieved by studies of adsorbate-induced surface structures. Copper catalysts are heavily used in methanol and formaldehyde synthesis, two reactions in which oxygen adsorption is an important intermediate step. To better understand catalytic reactions, it is imperative to both identify and characterize the atomic structure of all phases present on metal surfaces at elevated temperatures and pressures relevant to working catalysts. We will report on our discovery of a new high-temperature oxygen-induced surface phase on Cu (001) using a combination of in situ synchrotron x-ray scattering and first-principles theory. This high-temperature phase is characterized by 1/4 ML of randomly-distributed vacancies in the topmost Cu layer with a c(2x2)-O adlayer. Below 473 K a reversible transition to a $\left(2\sqrt{2} \times \sqrt{2}\right) R45^\circ$ missing row phase occurs. The results show that this entropy-driven phase transition occurs through the diffusion of Cu vacancies underneath the oxygen superstructure. This work is supported by DOE BES under Contract # DE-AC02-06CH11357.

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