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**Theoretical aspects of studies of high coverage oxidation of the Cu(100) surface using low energy positrons** N.G. FAZLEEV, W.B. MADDOX, J.A. REED, Department of Physics, University of Texas at Arlington — The study of adsorption of oxygen on transition metal surface is important for the understanding of oxidation, heterogeneous catalysis, and metal corrosion. The structures formed on transition metal surfaces vary from simple adlayers of chemisorbed oxygen to more complex structures which results from diffusion of oxygen into the sub-surface regions. In this work we present the results of an ab-initio investigation of positron surface and bulk states and annihilation probabilities of surface-trapped positrons with relevant core electrons at the Cu(100) missing row reconstructed surface under conditions of high oxygen coverage. Calculations are performed for various surface and subsurface oxygen coverages ranging from 0.50 to 1.50 monolayers. Calculations are also performed for the on-surface adsorption of oxygen on the unreconstructed Cu(001) surface for coverages up to one monolayer to use for comparison. Estimates of the positron binding energy, positron work function, and annihilation characteristics reveal their sensitivity to atomic structure of the topmost layers of the surface and charge transfer. Theoretical results are compared with experimental data obtained from studies of oxidation of the Cu(100) surface using positron annihilation induced Auger electron spectroscopy.

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