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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, 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 oxygen diffusion into the sub-surface region and the formation of oxides. 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 oxidized Cu(100) surface under conditions of high oxygen coverage. Calculations are performed for various high coverage missing row structures ranging between 0.50 and 1.50 ML oxygen coverage. 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. The geometry of the surfaces with adsorbed oxygen is fully optimized. 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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