Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Studies of high coverage oxidation of the Cu(100) surface using low energy positrons N.G. FAZLEEV, W.B. MADDOX, A.H. WEISS, Department of Physics, University of Texas at Arlington — The study of oxidation of single crystal metal surfaces is important in understanding the corrosive and catalytic processes associated with thin film metal oxides. The structures formed on oxidized transition metal surfaces vary from simple adlayers of chemisorbed oxygen to more complex structures which result from the diffusion of oxygen into subsurface regions. In this work we present the results of theoretical studies 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. The results of calculations of positron binding energy, positron work function, and annihilation characteristics of surface trapped positrons with relevant core electrons as function of oxygen coverage are compared with experimental data obtained from studies of oxidation of the Cu(100) surface using positron annihilation induced Auger electron spectroscopy (PAES).

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Date submitted: 23 Nov 2011 Electronic form version 1.4