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Studies of oxidation and thermal reduction of the Cu(100) surface using positron annihilation induced Auger electron spectroscopy

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Abstract

Positron annihilation induced Auger electron spectroscopy (PAES) measurements from the surface of an oxidized Cu(100) single crystal show a large increase in the intensity of the annihilation induced Cu M2,3VV Auger peak as the sample is subjected to a series of isochronal anneals in vacuum up to annealing temperature 300°C. The PAES intensity then decreases monotonically as the annealing temperature is increased to ~550°C. Experimental positron annihilation probabilities with Cu 3p and O 1s core electrons are estimated from the measured intensities of the positron annihilation induced Cu M2,3VV and O KLL Auger transitions. PAES results are analyzed by performing calculations of positron surface states and annihilation probabilities of the surface-trapped positrons with relevant core electrons taking into account the charge redistribution at the surface and various surface structures associated with low and high oxygen coverages. The variations in atomic structure and chemical composition of the topmost layers of the oxidized Cu(100) surface are found to affect localization and spatial extent of the positron surface state wave function. The computed positron binding energy and annihilation characteristics reveal their sensitivity to charge transfer effects, atomic structure and chemical composition of the topmost layers of the oxidized Cu(100) surface. Theoretical positron annihilation probabilities with Cu 3p and O 1s core electrons computed for the oxidized Cu(100) surface are compared with experimental ones. The obtained results provide a demonstration of thermal reduction of the copper oxide surface after annealing at 300°C followed by re-oxidation of the Cu(100) surface at higher annealing temperatures presumably due to diffusion of subsurface oxygen to the surface. © 2011 American Institute of Physics.

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Keywords

Annihilation, Auger, Beam, Copper, Oxidation, Positron, Spectroscopy