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Positron states and annihilation characteristics at the reconstructed (100) and (111) surfaces of Si with adsorbed hydrogen and oxygen. N.G. FAZLEEV, W.B. MADDOX, A.H. WEISS, Department of Physics, University of Texas at Arlington — We present results of theoretical studies of positron surface states, work functions and annihilation characteristics at the reconstructed (100) and (111) surfaces of Si with adsorbed hydrogen and oxygen. Calculations are performed taking into account geometrically optimized surface structures using a modified superimposed-atom method, and employing the corrugated-mirror model in a full three-dimensional geometry. The effects of adsorption of hydrogen and oxygen on the positron binding energy at the reconstructed (100) and (111) surfaces of Si and the positron work function are explored. The positron surface-state annihilation characteristics are computed for different hydrogen and oxygen coverages of both reconstructed surfaces of Si. The obtained results predict attenuation of the Si positron-annihilation-induced Auger electron signal intensity with the increase of the hydrogen and oxygen coverage consistent with experimental data. These studies confirm that positron-annihilation-induced Auger electron spectroscopy can be used to study changes in the properties of semiconductor surfaces due to the presence of adsorbed hydrogen and oxygen.

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