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Theoretical aspects of studies of oxide and semiconductor surfaces using low energy positrons

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Abstract

This paper presents the results of a theoretical study of positron surface and bulk states and annihilation characteristics of surface trapped positrons at the oxidized Cu(100) single crystal and at both As- and Ga-rich reconstructed GaAs(100) surfaces. The variations in atomic structure and chemical composition of the topmost layers of the surfaces associated with oxidation and reconstructions and the charge redistribution at the surfaces are found to affect localization and spatial extent of the positron surface-state wave functions. The computed positron binding energy, work function, and annihilation characteristics reveal their sensitivity to charge transfer effects, atomic structure and chemical composition of the topmost layers of the surfaces. Theoretical positron annihilation probabilities with relevant core electrons computed for the oxidized Cu(100) surface and the As- and Ga-rich reconstructed GaAs(100) surfaces are compared with experimental ones estimated from the positron annihilation induced Auger peak intensities measured from these surfaces.

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