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Image-potential surface states and positron annihilation characteristics at the reconstructed Si(100)-(2×1) and Si(100)-p(2×2) surfaces. N.G. FAZLEEV, J.L. FRY, A.H. WEISS, Department of Physics, University of Texas, Arlington — Positron probes of semiconductor surfaces are capable to non-destructively provide information that is both unique to the probe and complimentary to that extracted using other more standard techniques. In this talk the results of theoretical studies of positron surface states and annihilation characteristics of surface trapped positrons at the Si(100) surface are presented. Calculations are performed for the Si(100) surface with (2×1) and p(2×2) reconstructions. The orientation-dependent variations of the atomic density and electron density are found to affect the localization of the positron surface state wave function at the reconstructed surface. It is shown that the positron surface state wave function extends into the lattice in the regions where atoms are displaced from their ideal terminated positions due to reconstructions. Estimates of the positron binding energy and annihilation characteristics reveal their sensitivity to the specific atomic structure of the topmost layers of Si. The computed core annihilation probabilities are compared with the results of studies of Si(100) using Positron Annihilation Induced Auger Electron Spectroscopy (PAES). The sensitivity of annihilation probabilities to crystal face indicates that PAES could serve as an important surface diagnostic tool capable of distinguishing different semiconductor surfaces and defining their state of reconstruction.

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