Available online at www.sciencedirect.com
SCIENCE DIRECT
Applied Surface Science 252 (2006) 3333–3341
applied surface science
www.elsevier.com/locate/apsusc

Surface states and annihilation characteristics of positrons trapped at reconstructed semiconductor surfaces

N.G. Fazleev [a,b,*]

[a] Department of Physics, Box 19059, University of Texas at Arlington, Texas 76019-0059, USA
[b] Department of Physics, Kazan State University, Kazan 420008, Russian Federation

Available online 13 October 2005

Abstract

Positron probes of the Si(1 0 0) surface that plays a fundamental role in modern science and technology are capable to non-destructively provide information that is both unique to the probe and complimentary to that extracted using other more standard techniques. This paper presents a theoretical study of positron "image-potential" surface states and annihilation characteristics of surface trapped positrons at the Si(1 0 0) surface. Calculations are performed for the reconstructed Si(1 0 0)-p(2 × 2) surface using the modified superimposed-atom method to account for discrete-lattice effects, and the results are compared with those obtained for the non-reconstructed and reconstructed Si(1 0 0)-(2 × 1) and Si(1 1 1)-(7 × 7) surfaces. The effect of orientation-dependent variations of the atomic and electron densities on localization and extent of the positron surface state wave function at the semiconductor surface is explored. The positron surface state wave function is found to extend into the Si lattice in the regions where atoms are displaced from their ideal terminated positions due to the p(2 × 2) reconstruction. Estimates of the positron binding energy and positron annihilation characteristics reveal their sensitivity to the specific atomic structure of the topmost layers of Si. The observed sensitivity of annihilation probabilities to crystal face indicates that positron spectroscopy techniques could serve as an important surface diagnostic tool capable of distinguishing different semiconductor surfaces and defining their state of reconstruction.

Keywords: Silicon; Reconstruction; Surface; Positron; Localization; Annihilation

1. Introduction

Spatially extended "image-potential" electronic states near the surfaces of conductors have been intensely studied both theoretically and experimentally due to their role in surface phenomena and interest in quantum states of reduced dimensionality [1]. Like electrons, positrons can have surface-bound states localized in the region of the vacuum–medium interface [2]. These surface states are the consequence of the interplay between repulsion from the surface ionic cores and electron–positron correlations just outside the surface resulting in an attractive interac-

* Tel.: +1 817 272 2469; fax: +1 817 272 3637.
E-mail address: Fazleev@uta.edu.

0169-4332/$ – see front matter
doi:10.1016/j.apsusc.2005.08.082