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

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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-

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tion. Unlike the electron case, the ''image-potential'' surface states for positrons typically have lower energies than the bulk positron states, and these states form a trap for positrons that encounter the surface.

Positron surface states and annihilation characteristics of low energy positrons trapped at semiconductor surfaces are of interest because of the possibilities of using positrons in the development of new probes of surfaces, thin films, and nanostructures. Experimental studies of the nature and localization of the positron bound states at surfaces, both clean and adsorbate-covered, are currently performed using a surface characterization technique, positron annihilation induced Auger electron spectroscopy (PAES) [3].

The Si(1 0 0) surface continues to receive much attention, not only because of its technological importance, but also because it presents very rich physics related to its lattice reconstruction. In the unreconstructed situation, each surface atom would have two dangling bonds, which makes this geometry highly unstable. In consequence, the surface reconstructs by dimerization: pairs of Si atoms, originally at second nearest-neighbor positions, move to first nearest neighbor ones to form a covalent bond and to reduce the number of dangling bonds to one per surface atom. However, while the dimerization is a well-established fact both experimentally and theoretically, the geometry of the dimers and the atomic structure corresponding to the lowest energy remain a topic of important studies and a source of discussions. It has been found that when all dimers are similarly oriented, the Si(1 0 0) surface is characterized by a p(2 × 1) reconstruction in which rows of dimers are formed along the $[\bar{1}\,1\,0]$ direction. The alternation of buckling along dimer rows leads to a p(2 × 2) reconstruction. According to recently performed scanning tunneling microscopy studies [4] and theoretical analysis using the spin-unrestricted density functional theory and quantum Monte Carlo calculations [5] the buckled structure of the Si(1 0 0) surface corresponds to the one with the lowest energy.

The purpose of this paper is to perform theoretical studies of the positron surface state and positron annihilation characteristics at the reconstructed Si(1 0 0)-p(2 × 2) surface. Such studies are indispensable for clarifying the formation, stability, and localization of positron surface states at semiconductor surfaces. They also provide the surface structure dependence of positron annihilation characteristics, information needed for the interpretation of PAES studies.

2. Positron potential at a semiconductor surface

The potential due to a semiconductor surface felt by a positron $V^+(\boldsymbol{r})$ contains an electrostatic Hartree (Coulomb) potential $V_H(\boldsymbol{r})$ and a correlation part $V_{corr}(\boldsymbol{r})$. The Hartree potential $V_H(\boldsymbol{r})$ was constructed as a superposition of the atomic Coulomb potentials $V^{at}_{coul}(|\boldsymbol{r}-\boldsymbol{R}|)$ from all atoms located within a predetermined radius of the evaluation point, where $\boldsymbol{R}$ defines the positions of the host nuclei. Calculations of each bound electron state of the Si atom were performed self-consistently within the local-spin-density approximation [6] using the exchange-correlation functional and atomic configurations from references [7,8], respectively. The resulting wave functions are used to find the electron densities and corresponding atomic potentials via Poisson's equation.

In constructing $V_{corr}(\boldsymbol{r})$ at a semiconductor surface, we take into consideration the fact that the correlation component of $V^+(\boldsymbol{r})$ deep inside and far outside the semiconductor surface is described well using the local density approximation (LDA) and the image-type potential, respectively. It is possible then to divide space into two regions, namely the bulk and image potential regions, where the two models are applied. The border between these regions is chosen to pass through a crossover point of the bulk and image-type potentials, located outside the surface.

In the LDA, $V_{corr}(\boldsymbol{r})$ is obtained at a given position by considering the positron to be embedded in a homogeneous electron gas with an electron density n_- corresponding to the electron density at that particular point, i.e.:

$$V_{corr}(\boldsymbol{r}) = V^{LDA}_{corr}(\boldsymbol{r}, n_-) = V^{EG}_{corr}(n_-)[f(n_-, \epsilon_g)]^{1/3} \quad (1)$$

where $V^{EG}_{corr}(n_-)$ is the correlation energy of a positron in a homogeneous electron gas [9,10] of density n_-, $f(n_-,\epsilon_g)$ is a reduction factor which accounts for the diminished screening response of semiconductors to charged particles due to the existence of a band gap