



Influence of C-defect at Si(001) surface on the adsorption of Al, Ag and Pb atoms



B. Pieczyrak*, L. Jurczyszyn

Institute of Experimental Physics, University of Wrocław, pl. Maxa Borna 9, 50-204 Wrocław, Poland

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ABSTRACT

The influence of C-defect at Si(001) surface on the adsorption and aggregation of different kinds of metal ad-atoms is studied based on total energy and electronic structure density functional theory calculations. It was shown that the formation of C-defect by the dissociative adsorption of water molecule destroys π bonds in both silicon dimers incorporated into C-defect which leads to the appearance of unsaturated dangling bonds at the free ends of these dimers. The obtained results indicate that this process increases significantly the chemical reactivity of the substrate surface in front of C-defect for three different metallic ad-atoms: Al (III group), Pb (carbon group) and Ag (transition metal). It was shown that the increase of the adsorption energy in the vicinity of C-defect can initiate the process of aggregation of ad-atoms diffusing on silicon substrate.

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1. Introduction

The ad-atoms of groups III and IV diffusing on the Si(001) substrate tend to aggregate in the form of chain-like structures. For more than a decade the formation of such ordered structures has been investigated intensively *via* experimental and theoretical approaches [1–15]. The knowledge about the physics controlling this one-dimensional aggregation plays a crucial role in adopting the specific properties of such low-dimensional structures for nano-technological applications. The scanning tunneling microscopy (STM) and spectroscopy (STS) measurements are the source of valuable information related to different aspects of this kind of aggregation.

In the case of Si(001) substrate three types of surface defects (A, B and C) are frequently observed. A and B-type of such defects are interpreted as the one or two missing dimers, respectively. In the case of C-defect it was shown independently by Hossain et al. [16] and Okano and Oshiyama [17] that it represents the product of the dissociative adsorption of water molecule. Following this idea, C-defect is composed of H atom and hydroxyl group bonded to neighboring Si atoms of two adjacent surface dimers from the same row.

It was shown that C-defect significantly increases the local chemical reactivity of Si(001) substrate – the experimental and theoretical studies [6,7,18] indicate that C-defect can stabilize the position of In ad-atoms diffusing on Si(001) and initiate the formation of chain-like structures composed of such ad-atoms. These structures are oriented perpendicular to the rows of surface dimers at Si(001) substrate and pinned by one of its ends to C-defect. The comparison of the bonding of ad-atoms from the III group such as In, Ga and Al with C-defect has been presented in earlier theoretical study [19].

The aim of our present study is to check if C-defect can also influence the adsorption of other types of metal ad-atoms. We have considered here three kinds of metal ad-atoms such as Al (metal from III group), Pb (carbon group) and Ag (transition metal). In the framework of our theoretical study we have compared the adsorption energies of these ad-atoms at the clean Si(001) with the corresponding values obtained for the ad-atom adsorption at C-defect, to answer if C-defect can initiate the aggregation also for ad-atoms different than ad-atoms from III group. Moreover, we have also shown that C-defect increased significantly the adsorption energy of Si ad-atom. The obtained results let us clarify some points responsible for the increase of the local chemical reactivity by C-defect.

2. Method of calculation

In the framework of our theoretical study we have performed *ab initio* structural calculations based on the density functional theory

* Corresponding author. Tel.: +48 713759343.
E-mail address: meghan@ifd.uni.wroc.pl (B. Pieczyrak).

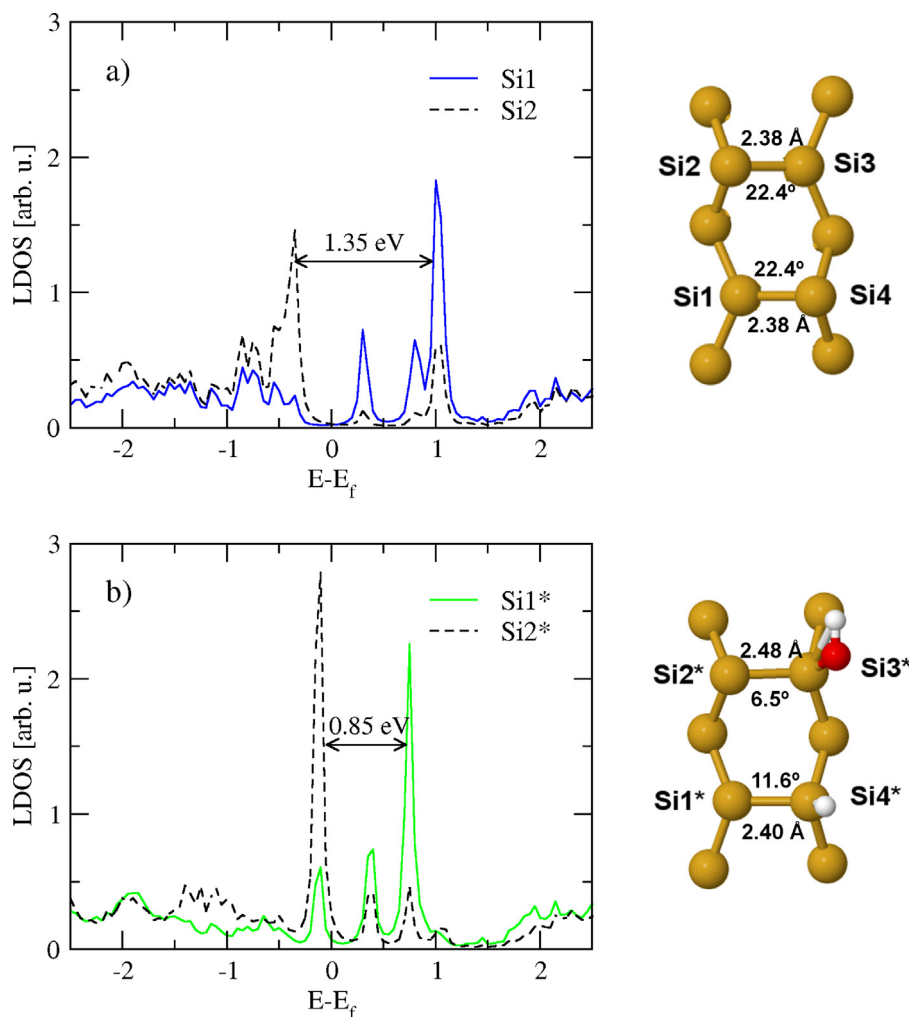


Fig. 1. Calculated local density of states at clean Si(001) surface (a) and at Si(001) surface with C-defect (b). Corresponding atomic structures in top view are also shown on the right side.

(DFT) where the ion cores were described by norm-conserving pseudopotentials and the exchange-correlation contributions were introduced by local-density-approximation (LDA). In these calculations the electronic wave functions were constructed using pseudoatomic, slightly excited spd orbitals (code Fireball) [20,21]. In these calculations we use a minimal basis set of numerical atomic orbitals with the following cut-off radii (in a.u.): $s=4.8$, $p=5.4$, $d=4.6$ (Si); $s=3.3$, $p=3.8$ (O); $s=4.0$, $p=4.5$ (C); $s=3.8$ (H); $s=5.3$, $p=5.7$ (Al); $s=5.3$, $p=5.7$, $d=4.5$ (Ag); $s=4.8$, $p=5.7$, $d=4.8$ (Pb). The total energy calculations have been performed for the system where the silicon substrate was described by an asymmetric slab using 8×6 unit cell and built up of six atomic layers: the position of atoms in the bottom layer were fixed and the dangling bonds were saturated by H atoms. The relaxation of atomic positions has been performed using the combination of conjugate gradient and dynamical quenching algorithms until the forces were below 0.05 eV/\AA . The surface Brillouin zone was sampled by two k-points.

3. Results and discussion

3.1. C-defect – structural and electronic properties

In the first step we have considered the structural and electronic properties of the single C-defect on Si(001). C-defects are commonly observed on Si(001) substrate, however their origin

and physical nature are still a source of controversy. The recent STM measurements as well as theoretical considerations strongly support the opinion that C-defect originates from the dissociative adsorption of single water molecule. Following this model, C-defect is produced by the hydrogen atom and hydroxyl group dissociated from water molecule and adsorbed on the same side of two adjacent silicon dimers along the dimer row.

At low temperature, Hata et al. [22] observed two types of C-defects: semiconducting and metallic C-defect. These two types could not be distinguished at RT. However, previous *ab initio* calculations [7] have shown that semiconducting or metallic C-defect leads to very similar results. Therefore, our present theoretical study is limited only to the metallic C-defect.

The results of the structural calculations indicate that the adsorption of hydrogen and hydroxyl group leads to the destruction of π bonds in both silicon dimers in C-defect which leads to the appearance of the unsaturated dangling bonds at the free ends of these dimers. As a result, the length of both dimers from the C-defect is considerably enlarged: from 2.38 (clean surface) to 2.48 Å – dimer with hydroxyl group and 2.4 Å – dimer with hydrogen. This effect is associated with the reduction of the dimer buckling: from 22.4° (clean surface) to 11.6° – dimer with hydrogen and 6.5° – dimer with hydroxyl group. Fig. 1 shows the comparison of the LDOS distribution associated with two ends of two subsequent silicon dimers along dimer row at the clean Si(001) substrate with the corresponding distributions calculated for the free ends of the

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