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# Spin-splitting band dispersions of the heavy elements on Si(111)–(1×1) surface

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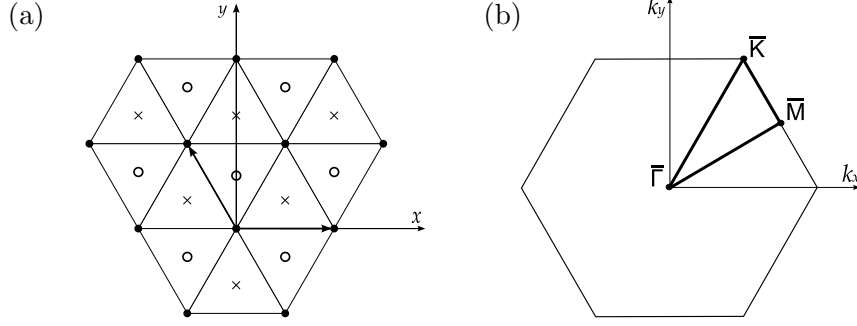
## Abstract.

We have carried out the first-principles fully relativistic electronic structure calculations for the surfaces,  $R/\text{Si}(111)$  ( $R = \text{Pb}$  and  $\text{Bi}$ ). The band dispersions of the surface states in the bulk band gap shows the large spin splitting, associated with the spin-orbit interaction on the atoms of the overlayer. Besides the usual Rashba effect around the center of the surface Brillouin zone, the vortical spin polarizations were obtained around the  $\bar{M}$  points. At the  $\bar{K}$ , associated with the symmetry, the complete out-of-plane spin polarization was obtained for the surface states.

## 1. Introduction

The recent development on the experimental measurements of high-resolution angle-resolved photoelectron spectroscopy (ARPES) and its spin-polarized (SP) version has allowed one to obtain the spin splitting of surface band dispersions [1, 2]. Such phenomena appear as Rashba effects, which are originated by the spin-orbit interaction (SOI) on electrons. These effects have been increasing variations of the interest to spin manipulation in spin electronics (spintronics) devices [3]. For the ideal two dimensional electron, which is moving in the potential gradient along  $z$ -direction, the electron spin with  $\vec{k}$  is polarized along the direction of  $\vec{e}_z \times \vec{k}$ , which forms a vortical spin configuration around  $\bar{\Gamma}(\vec{k} = 0$  in the surface Brillouin zone (SBZ)). Such a vortical spin polarization has been obtained also around the  $\bar{M}$  point of the SBZ for  $\text{Tl}/\text{Si}(111)\text{--}(1\times 1)$  surface by the theoretical study [4]. The rotation of spin from the in-plane direction of surface has been discussed around  $\bar{\Gamma}$  [3]. Furthermore, the definitive perpendicular polarization with respect to the surface plane has been observed by SP-ARPES and confirmed by the first-principles calculations [4]. In the previous report, however, the descriptions about the symmetry and the group theory did not cover any detail of electronic states.

In this report, besides the case of Tl overlayer, we present the analysis of band structures for the overlayers of Pb and Bi on Si(111) surface with  $1 \times 1$  configuration. The Pb and Bi systems have not been obtained as the stable and meta-stable surface [5, 6, 7, 8, 9], however, there are surface bands in the bulk band gap of Si and, the spin splittings and the spin polarizations at the  $\mathbf{k}$  points far from the  $\bar{\Gamma}$  can easily be discussed, compared with the Tl system and the results of the group theory.



**Figure 1.** Schematic diagram of  $R/\text{Si}(111)-(1\times 1)$  surface (a) and surface Brillouin zone (b). The open and filled circles specify the atoms of  $R$  and  $\text{Si}(1)$  (the  $\text{Si}$  atom in the top layer), respectively, and the crosses the other high symmetry points in (a).

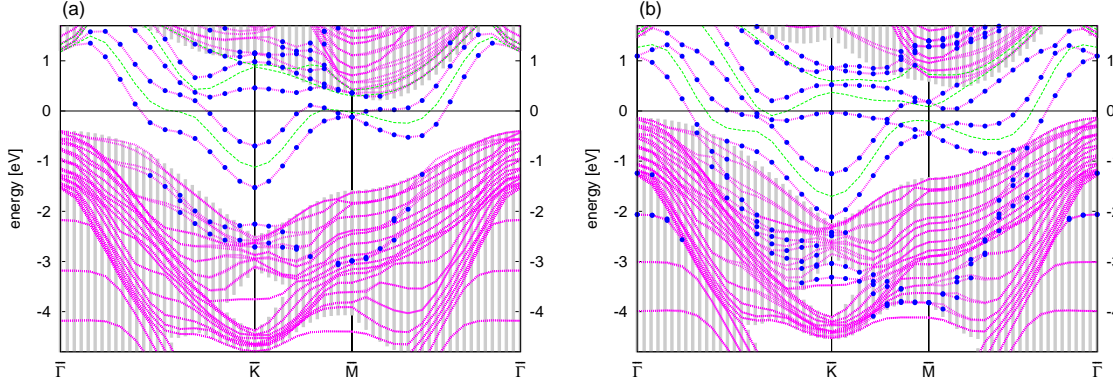
**Table 1.** Symmetry-adapted atomic basis functions of spinor  $p$ -orbitals on the  $R$  site for the groups at  $\bar{\Gamma}$ ,  $\bar{K}$ , and  $\bar{M}$ . The label  $\Gamma_n$  specifies the irreducible representation of each group.

$\mathbf{k}$	representation	$R$ site
$\bar{\Gamma}$	$\Gamma_4, \Gamma_5$	$\begin{pmatrix} a_1(x+iy) \\ a_2(x-iy) \end{pmatrix}, \begin{pmatrix} -a_2^*(x+iy) \\ a_1^*(x-iy) \end{pmatrix}$
	$\Gamma_6$	$\left\{ \begin{pmatrix} a_3z \\ a_4iz \end{pmatrix}, \begin{pmatrix} a_4iz \\ a_3z \end{pmatrix} \right\}, \left\{ \begin{pmatrix} a_5(x+iy) \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ a_5(x-iy) \end{pmatrix} \right\}$ $a_3, a_4, a_5$ : real number
$\bar{K}$	$\Gamma_4, \Gamma_5, \Gamma_6$	$\begin{pmatrix} b_1z \\ b_2(x+iy) \end{pmatrix}, \begin{pmatrix} b_3(x-iy) \\ b_4z \end{pmatrix}, \begin{pmatrix} b_5(x+iy) \\ b_6(x-iy) \end{pmatrix}$
$\bar{M}$	$\Gamma_3$	$\begin{pmatrix} c_1z + c_2(\frac{\sqrt{3}}{2}x + \frac{1}{2}y) + c_3(-\frac{1}{2}x + \frac{\sqrt{3}}{2}y) \\ c_4z + c_5(\frac{\sqrt{3}}{2}x + \frac{1}{2}y) - c_3(-\frac{1}{2}x + \frac{\sqrt{3}}{2}y) \end{pmatrix}$
	$\Gamma_4$	$\begin{pmatrix} -c_4^*z - c_5^*(\frac{\sqrt{3}}{2}x + \frac{1}{2}y) + c_3^*(-\frac{1}{2}x + \frac{\sqrt{3}}{2}y) \\ c_1^*z + c_2^*(\frac{\sqrt{3}}{2}x + \frac{1}{2}y) + c_3^*(-\frac{1}{2}x + \frac{\sqrt{3}}{2}y) \end{pmatrix}$
$\bar{K}$	$\Gamma_1, \Gamma_2, \Gamma_3$	$d_3z, d_1(x+iy), d_2(x-iy)$ $\Gamma_4 + \Gamma_6 \longrightarrow \Gamma_2, \Gamma_5 + \Gamma_6 \longrightarrow \Gamma_3, \Gamma_4 + \Gamma_5 \longrightarrow \Gamma_1$

## 2. Two dimensional space group $p3m1$ and surface Brillouin zone

The system of  $R/\text{Si}(111)-(1\times 1)$  surface has the symmetry operations ;  $C_3$  (three-fold rotation) and  $m$ (mirror line). The two dimensional space group formed in such a system is identified by the crystallographic international symbol of  $p3m1$ . This group is distinguished with  $p31m$ . The schematic diagram of the real lattice is presented in figure 1(a). In figure 1(b), the SBZ is shown with the symbols of symmetry point. The typical  $\mathbf{k}$  groups are  $C_{3v}$ ,  $C_3$ , and  $C_{1h}$  for  $\bar{\Gamma}$ ,  $\bar{K}$ , and  $\bar{M}$ , respectively. For the  $\bar{\Gamma} - \bar{M}$  line, the  $\mathbf{k}$  group is  $C_{1h}$  and the  $\bar{\Gamma} - \bar{K}$  does not have any geometrical symmetry.

Though the point of  $\bar{K}$  has the high symmetry, the spin splittings are observed because all the irreducible representations associated with  $\bar{K}$  are one dimensional and the time reversal symmetry does not create any degeneracy at the same  $\bar{K}$ . It is interesting to see that at the  $\bar{K}$  the spin direction can be polarized along the  $z$ -direction (the surface normal). In table 1, the atomic basis functions at  $\bar{\Gamma}$ ,  $\bar{M}$ ,  $\bar{K}$  are presented for  $R$  site. For  $\bar{K}$ , the functions with neglecting the SOI are also shown.



**Figure 2.** (color online) Band dispersions of  $R/\text{Si}(111)-(1 \times 1)$  surface (a)  $R = \text{Pb}$  (b)  $R = \text{Bi}$ . The bullets on the dispersion curves (thick curves) specify a large component of  $R$  6p orbitals. The hatched area with the vertical bars means the bulk band projection of Si. Thin dashed curves are from the selected dispersions without the spin-orbit interaction. The horizontal lines specify the Fermi level.

### 3. Electronic structures of $R/\text{Si}(111)$

#### 3.1. Methods and models

The electronic structure calculation has been performed by means of an ultrasoft pseudopotential plane-wave method [10]. The method used includes the fully relativistic effect, which contains the SOI, through the relativistic version of pseudopotentials [11]. The generalized gradient approximation was used. The energy cutoffs of 25 and 300 Ry for wavefunctions and charge densities were taken [10]. The surface system was modeled by the repeated slab for calculation, which have a  $R$ -monolayer (ML), 16 Si-MLs, a H-ML, and the vacuum space more than 9 Å.

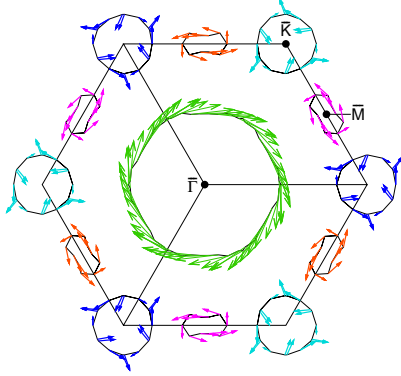
The  $1 \times 1$  configuration on Si(111) surface has three adsorbing typical sites; T1, H3, and T4 sites. In the Tl/Si(111)-(1×1), the T1 model is much higher in energy than the H3 and T4 models. These latter have similar energies respectively; the H3, in which each Tl atom has three neighboring Si atoms, is slightly higher in energy by 85 meV/Tl than the T4 in which has four neighboring Si atoms. The T4 site model is consistent with the ARPES measurements [4, 12] for Tl/Si(111)-(1×1). In this paper the T4 site model is used for the overlayers;  $R = \text{Pb}$ , and Bi, showing effects of the atomic number.

#### 3.2. Band dispersions

In vicinity of the Fermi level the surface band dispersions appear, as shown in figures 2(a) and 2(b) for Pb and Bi, respectively. The maximum SOI splitting is observed at  $\bar{K}$ , amounting to 0.82 eV for the splitting of  $\Gamma_4 - \Gamma_6$  ( $E(\Gamma_4) = -1.52$  eV,  $E(\Gamma_6) = -0.70$  eV) in the Pb system and 0.86 eV for  $\Gamma_4 - \Gamma_6$  ( $E(\Gamma_4) = -2.11$  eV,  $E(\Gamma_6) = -1.25$  eV) in the Bi system.

The  $R$ -atom orbital components which appear in the gap of the bulk projection move to a lower range in energy as the atomic number increases. The band dispersions measured in the Tl/Si(111) appear just above the valence band area of the bulk projection [4], while the corresponding bands in  $R = \text{Pb}$  and Bi were found to sink almost in the bulk band.

The eigenstate with SOI determines the spin polarization vector  $\vec{\sigma}_n(\vec{k})$  of the state with the wave vector  $\vec{k}$ ;  $\vec{\sigma}_n(\vec{k}) = \langle \varphi_{n\vec{k}} | \vec{\sigma} | \varphi_{n\vec{k}} \rangle_R$ , where  $\vec{\sigma}$  is Pauli's spin matrix. At  $\bar{K}$  the  $\vec{\sigma}_n(\vec{k})$  has only a  $z$ -component. Around  $\bar{\Gamma}$  and  $\bar{M}$ , as in the usual Rashba effect, the  $\vec{\sigma}_n(\vec{k})$  has a vortical spin configuration. As a typical one, the projected diagram of  $\vec{\sigma}_n(\vec{k})$  is shown at the fixed energy states in figure 3. In this energy level, there are three kinds of constant energy lines; around  $\bar{\Gamma}$ ,



**Figure 3.** (color online) Spin polarizations projected onto the  $xy$  plane in the surface Brillouin zone for the states which have the energy of  $E - E_F = -0.22\text{eV}$  in Pb/Si(111)-(1 $\times$ 1) surface. The spins around  $\bar{K}$ s are exaggerated by the factor of four compared with those around  $\bar{\Gamma}$  and  $\bar{M}$ s.

$\bar{M}$  and  $\bar{K}$ . Around  $\bar{\Gamma}$ , the clockwise polarizations are observed and at the same time, around  $\bar{M}$  the anti-clockwise.

#### 4. Summary

We have investigated electronic structures of the lead and bismuth overlays on Si(111)-(1 $\times$ 1) surface with using a first-principles approach of the fully relativistic spinor-planewave method. The large spin splittings associated with the SOI were obtained in bulk band gap. The vortical spin polarizations were observed around both  $\bar{\Gamma}$  and  $\bar{M}$ . The spin polarization along the surface normal was obtained at the surface states of  $\bar{K}$  in the SBZ. These conclusions await experimental investigations about the symmetry-adapted systems other than the Tl system.

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