Project of collaboration Sydney-Liverpool. Stay of Dr. Lin at The University of New South Wales: A complete description of electron tunneling transport in the P doped Si surfaces

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1 Purpose of the visit

The fabrication of atomic-scale devices in silicon often requires the encapsulation of dopant atoms. In this way, the delicate nano-devices can be well protected while the modification of surface states due to the dopant atoms is remained [1, 2, 3]. Very interestingly, the dopant states has been demonstrated very sensitive to the bias voltage in STM operations. Since the doped silicon surfaces are regarded as important templates for a wide range of applications in nano-scale devices, a thorough understanding how dopant atoms influence the electronic structure at the atomic level will play a crucial role in designing and fabricating microscopic electronic devices in future. To date, however, the theoretical interpretations of STM images of doped semiconductor surfaces has been missing due to the lack of knowledge of tunneling mechanism at the interfaces and inside the leads (surface and tip). In this collaboration, we are aiming at a reliable STM code for calculating coherent electron transport in a complete STM imaging processes (substrate-interface-vacuum-interface-tip).

The project is based on the density functional theory calculations implemented in the GPAW package [4]. In the first step, the electronic structures of surface, tip, surface bulk and tip bulk are characterized from accurate DFT calculations. The resulted wave functions (Bloch states) can then be represented by maximally-localized Wannier functions. The localized basis functions together with the obtained effective potentials can then be employed to construct the Green's functions (g_{TT} and g_{SS}) of the semi-infinite surface and tip systems. We assume that the Green's functions of tip and surface does not change during the STM imaging process. Thus, for each tip-surface configuration, in the combined system, the tip-surface coupling (V_{TS} and V_{ST}) can be calculated by

$$V_{TS} = \langle \phi_i | V_{eff} + \nabla^2 | \phi_j \rangle \tag{1}$$

where $V_{eff} = V_S + V_T$ while ϕ_i and ϕ_j are the localized basis functions of tip and surface respectively.

$$V_{ST} = V_{TS}^{\dagger} \tag{2}$$

The current value is then given by:

$$I = \int d\omega (f_S - f_T) Tr[V_{ST} \alpha_{TT}(\omega) V_{TS} \alpha_{SS}(\omega)], \tag{3}$$

where

$$\alpha_{TT} = g_{TT} - g_{TT}^{\dagger} \text{ and } \alpha_{SS} = g_{SS} - g_{SS}^{\dagger}. \tag{4}$$

2 Description of the work carried out during the visit

2.1 Construction of the semi-infinite leads

In this project, the STM tip used in all calculations is modeled by a W(111) slab with a small pyramid. The super cell extends periodically in three dimensions. A vacuum of 15 Å is used to separate the periodic images in z direction, see Fig.1 (a). The W atoms in the small pyramid is allowed to relax until the forces on each atom is smaller than 0.01 eV/Å. The electronic property of the tungsten bulk is calculated with a W slab shown in Fig.1 (b).

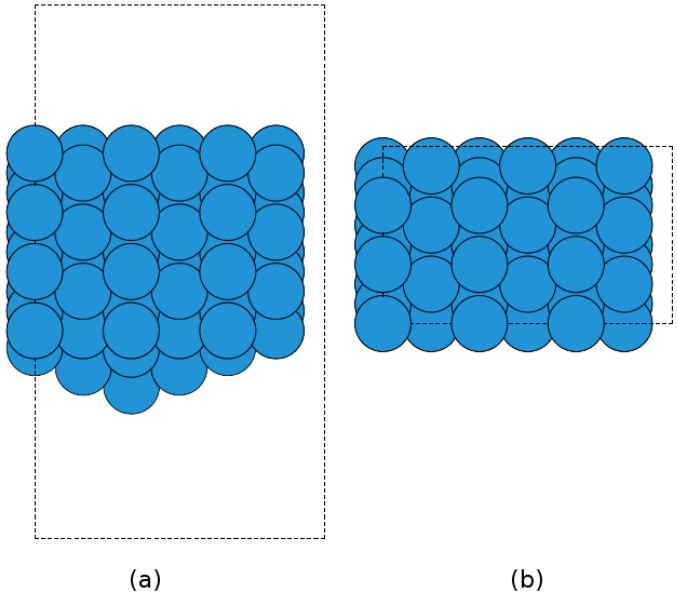

Figure 1: (a) Structure of a W(111) tip in DFT calculation, (b) Structure of a W slab used for electronic structure calculation of tungsten bulk.

In Fig.1 (a), the atoms of the periodic tungsten layer in the middle of the unit cell are regarded to have similar electronic properties as the atoms in the bulk. We call these periodic layer a principal layer. The atoms close to the tip surface are referred as on-site atoms see Fig.1 (a). The Hamiltonian of the on-site atoms and the principal layer is denoted to H_0 and H_1 respectively. If the size

of principal layer is properly selected so that all principal layers couple only with their nearest neighbours, a semi-infinite tip can be constructed as shown in Fig.2 (b). The Hamiltonian of the semi-infinite tip can therefore be written

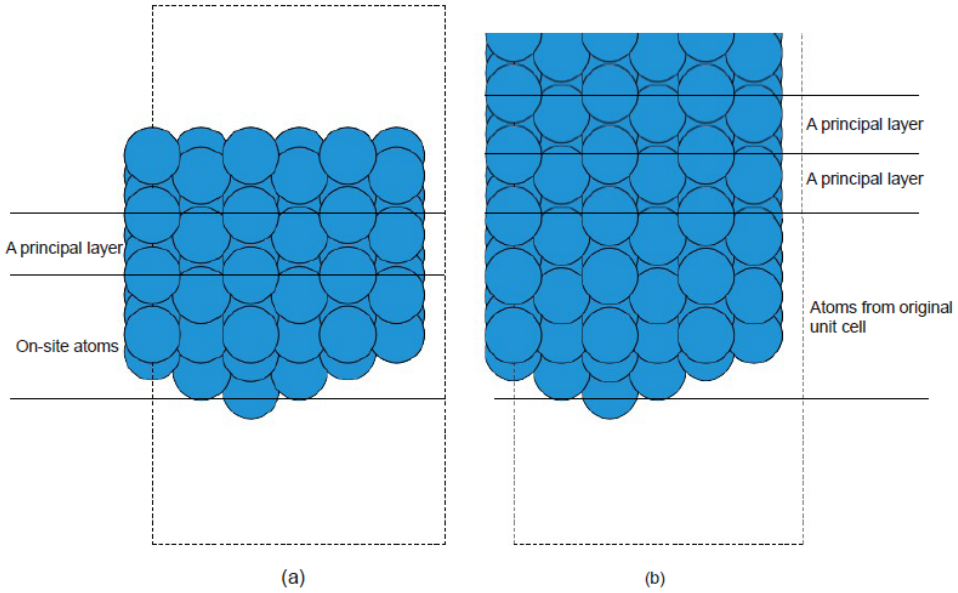

Figure 2: (a) The tungsten atoms which have similar electronic properties as the bulk atoms are referred as a principal layer. The atoms close to the surface are called on-site atoms. (b) A semi-infinite W(111) tip is constructed by using on-site atoms from original tip calculation and an infinite number of principal layers.

as

$$\mathbf{H} = \begin{pmatrix} \mathbf{H}_0 & \mathbf{V}_{10}^{\dagger} & 0 & 0 & \dots \\ \mathbf{V}_{10} & \mathbf{H}_1 & \mathbf{V}_{11}^{\dagger} & 0 & 0 \\ 0 & \mathbf{V}_{11} & \mathbf{H}_1 & \mathbf{V}_{11}^{\dagger} & 0 \\ 0 & 0 & \mathbf{V}_{11} & \mathbf{H}_1 & \mathbf{V}_{11}^{\dagger} \\ \vdots & 0 & 0 & \mathbf{V}_{11} & \ddots \end{pmatrix}. \tag{5}$$

Here, $\mathbf{H}_0$ and $\mathbf{H}_1$ refer to the Hamiltonian matrix of the on-site atoms and principal layer atoms respectively. $\mathbf{V}_{10}$ and $\mathbf{V}_{11}$ represent the coupling of the on-site atoms and the first principal layer and interactions between two nearest principal layers. The Green's function of this semi-infinite system can thus be expressed as

$$\mathbf{G}^r(\epsilon) = (z\mathbf{S}_0 - \mathbf{H}_0 - \mathbf{\Sigma}^r(\epsilon))^{-1}, \tag{6}$$

the matrix Σ^r is the self energy which incorporates the coupling of principal layers to the on-site part of the system.

$$\mathbf{\Sigma}^r(\epsilon) = (z\mathbf{S}_{0\alpha} - \mathbf{H}_{0\alpha})\mathbf{g}^r_\alpha(\epsilon)(z\mathbf{S}^\dagger_{0\alpha} - \mathbf{H}^\dagger_{0\alpha}) \tag{7}$$

Here, $\mathbf{S}_{0\alpha}$ and $\mathbf{H}_{0\alpha}$ are the coupling of Hamiltonian and overlap matrix and $\mathbf{g}^r_\alpha(\epsilon)$ is the Green's function of at the interface of on-site atoms and the first principal layer.

$$\mathbf{g}^r_\alpha(\epsilon) = (z\mathbf{S}_\alpha - \mathbf{H}_\alpha)^{-1} \tag{8}$$

The value of $\mathbf{g}^r_\alpha(\epsilon)$ can be calculated iteratively.

There are two P doped Si surfaces used for STM simulations. The first one is a single P doped Si(001) slab with (2x1) reconstruction, i.e. reduce half of the dangling bonds by forming dimers at the exposed surface, see Fig. 3 (a). The other is hydrogen terminated Si(001) surface with one P atom in the same atomic position, see Fig. 3 (b). The P atoms in both surfaces are four atomic layer (around 5 Å) below the top surface atoms. Similar to the W(111) tip, semi-infinite surface leads are also constructed by stacking principal layers below on-site atoms.

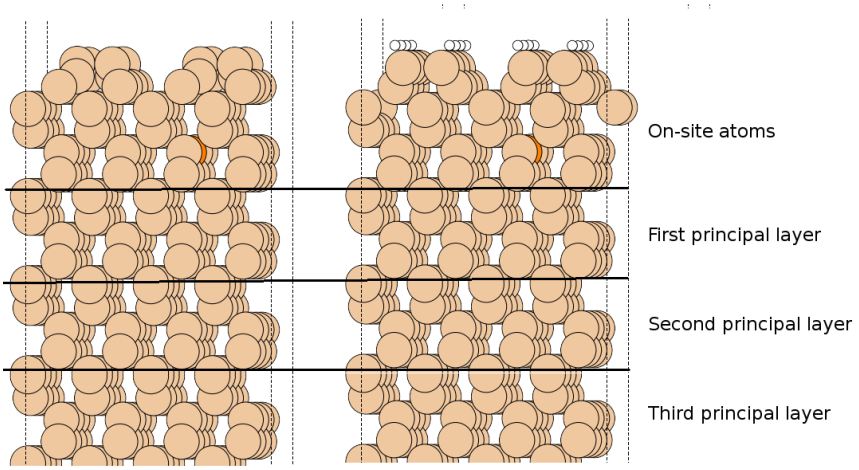

Figure 3: (a) Structure of a P doped Si(001)-2x1 reconstruction surface (b) Structure of hydrogen terminated P doped Si(001) surface

2.2 Experimental observations

The STM image of buried phosphorus atoms near Si(001)-(2x1) surface is shown in Fig.4 (a) and (b). The two images were taken sequentially in the same surface area. The bright feature in Fig.4 (a) is attribute to the subsurface P dopants. Fig.4 (b) exclude the possibility of surface defects, indicating that the peak in Fig.4 (a) arises from a subsurface feature [5]. However, the detailed atomic positions of dopant atoms are unknown.

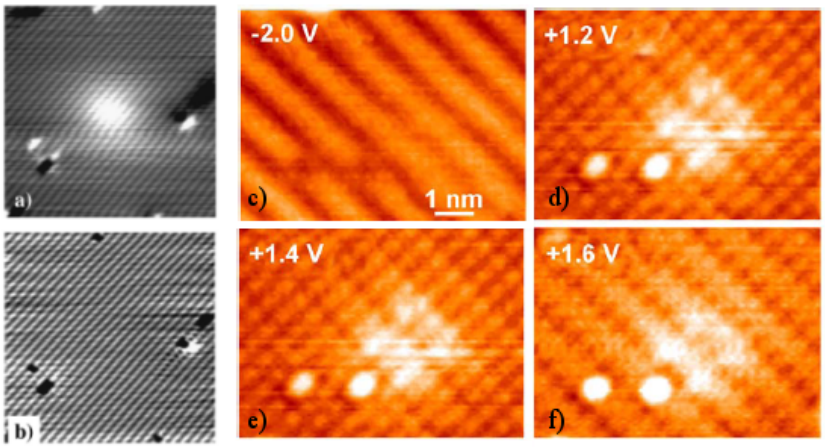

Figure 4: (a) and (b) are filled-state images of buried P atoms in Si(001)-(2x1) (a) V = -0.6V, I = 0.11nA, image area: (b) V = -1.5V, I = 0.11nA. (c)-(f) are STM images of P dopant under hydrogen terminated Si(001) surfaces at sample bias voltages of -2.0V, 1.2V, 1.4V, 1.6V, I = 0.13nA

Fig.4 (c)-(f) are STM images of P dopants under hydrogen terminated Si(001) surfaces. As can be seen, the dopant states in filled state STM image at -2.0V shows a very faint increase in intensity. However, at positive sample bias voltages, the P states are imaged as a big bright peak. In addition, the apparent height of the bright feature respect to the hydrogen-terminated Si dimmer increases as the sampled bias decreases from +1.6V to +1.2V [3].

2.3 STM simulation with other method

The existing STM simulation codes are using either Tersoff-Hamnann method [6, 7] or Bardeen's approach [8]. In order to demonstrate the uniqueness of our new STM code, I performed STM simulation with both existing methods on the Si surfaces shown in Fig. 3. As we expected, the dopant state is invisible if we take only the tunneling in the vacuum into consideration. In addition, the apparent height of P doped surface is identical to the clean Si surface.

2.4 STM simulation with new method

P doped Si(001)-(2×1)

STM simulations at -1.6V bias voltage of a clean Si(001)-(2x1) surface and a single P doped Si(001)-(2x1) surface are shown in Fig. 6. As can be seen, the P atom results in a non-local enhancement of the tunneling current. This fit quite well with experimental observations, see Fig. 4 (a). Although STM experiments indicate that this enhancement affects an area of 60×60 Å, due to the size limit of DFT calculation, exact decay length was not evaluated in this project. The

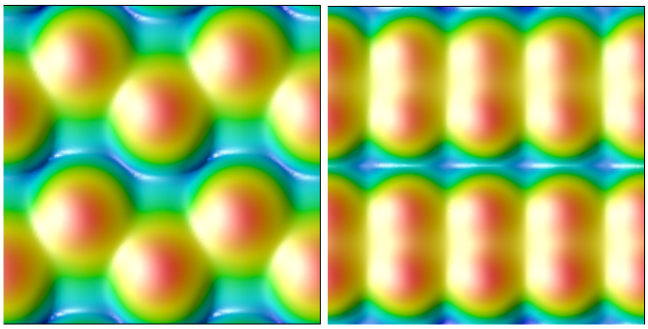

Figure 5: STM simulation of filled-state images of a single buried P atom below (a) Si(001)-(2x1) and (b) Hydrogen terminated Si(001) surface. The simulated image using Tersoff-Hamnann method and Bardeen's approach is the same: no dopant states can be imaged

same simulations have also been performed at -0.6V bias voltage. However, the

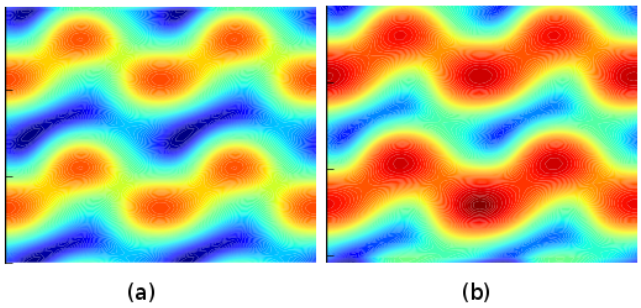

Figure 6: STM simulation of filled-state images of (a) a clean Si(001)-(2x1) surface (b) a single P atom doped Si(001)-(2x1) surface using Green's functions. V = -1.6V

very faint enhancement due to dopant atom (Fig. 4 (b)) was not reproduced. In contrast, as the absolute value of bias voltage increases, the apparent height of the bright feature increases as well. From experiments, we know that the P atom should be much more deeper (a few nanometers) below the surface than it is in 3 (a). Since the electronic structure at surface varies for different doping configurations, this mismatch of bias voltage dependency is attributed to the unknown atomic structure of doped Si surface.

P dopant below a hydrogen terminated Si(001)

STM simulations of buried P below hydrogen terminated Si(001) surface are shown in Fig. 7. As can be seen, for the empty states STM simulation (Fig.

7 (b)), the bright feature arises due to the dopant states. This is consistent with Fig. 4 (f). However, the apparent height of this bright feature does not decrease as we change bias voltage from +1.2V to +1.6V. Nevertheless, for filled states, the enhancement become fade out, which fit quite well with experimental results, see Fig. 7 (a).

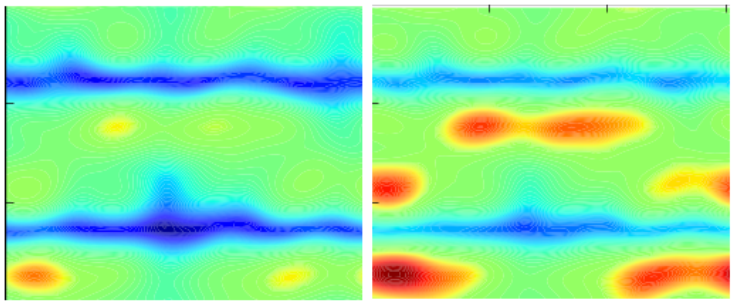

Figure 7: STM simulation of empty-state images of a single P atom doped Si(001) surface covered with H using Green's functions. (a) V = -2.0V (b) V = 1.6V

Summary

With the two testing systems, we proved that our new STM code is able to image the dopant states a few Angstroms below the Si surface. The simulated images fit with experimental observations.

3 Projected publications/articles resulting or to result from the STSM

Since at the present stage, our new STM simulation code can be considered finished and the computational approach working efficiently. The documentation of our implementation could be of interest for the computational Solid State Physics community. In addition, successful STM simulations on buried dopant atoms below semiconductor surfaces has not been achieved before. We therefore going to publish our simulation results as soon as possible.

References

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