Edge Reconstruction and Edge States in Ultrathin Sb(110)

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1. Introduction

Sb has been intensively studied recently due to its unique topological surface states[1]. The studies mainly focus on Si(111) surface. Since Sb(110) surface is not the cleavage plane of Sb, it is rarely studied. We report the first studies of ultrathin Sb(110) from 2 to tens of ML, that are prepared on HOPG. The Sb(110) follow even-ML growth mode below 6 ML. above 6 ML, both even- and odd-ML Sb(110) can be observed. First-principles calculations showed that the Sb(110) is relaxed, unlike the case of Sb(111) thin film, which is bulk-like. 4 × 1 reconstruction on the edge of ultrathin Sb(110) are found to form under certain conditions. Possible model for the 4 × 1 edge reconstruction is proposed.

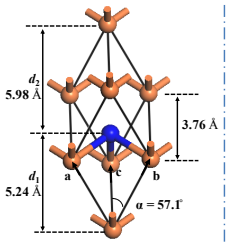
2. Experimental and computational methods

❖Experiments were performed in Unisoku LT-STM system. Sb atoms were deposited onto HOPG substrate held at RT, with chamber pressure kept below 3×10^{-10} mbar. Then sample was transferred to STM stage at 77 K.

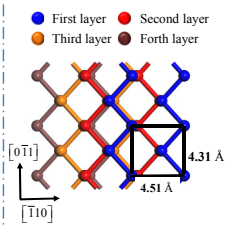
❖Energies and atomic structures of Sb(110) thin film were calculated by first-principles DFT method, using Vienna Ab-initio Simulation Package.

3. Results and discussions

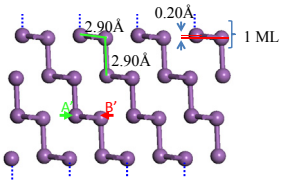
Bulk Sb atomic structure



Bulk Sb rhombohedral unit cell. Three base vectors are marked as **a**, **b** and **c**.

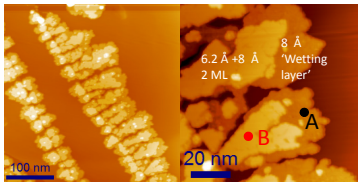


Top view of bulk terminated Sb(110)

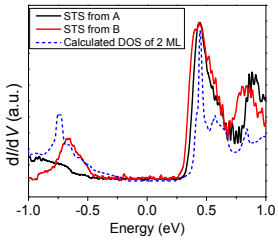


Side view of 4 ML bulk terminated Sb(110) from $[01\bar{1}]$ direction . Blue dash lines indicate dangling bonds.

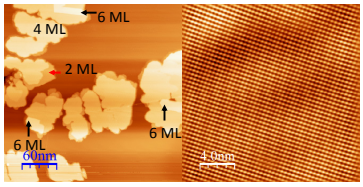
Sb growth mode on HOPG



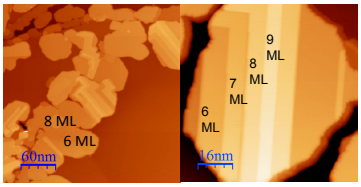
2.2 ML Sb deposited onto HOPG. Islands grown along the HOPG edge. The 8 Å height layer is treated as wetting layer since it does not contribute to the STS compared with calculated DOS. See right Fig.



Calculated DOS of 2 ML Sb(110) is much like STS from point B rather from point A.

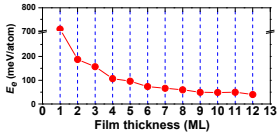


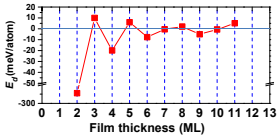
5.0 ML Sb deposited onto HOPG. 2, 4, 6 ML Sb(110) can be observed. **No 1, 3, 5 ML** can be found. Right Fig. is the atomic-resolution STM image on 4 ML Sb(110)



8.6 ML Sb deposited onto HOPG. **Above 6 ML, both even- and odd-ML Sb(110) exist.**

Why no 1, 3 and 5 ML? Calculated energy



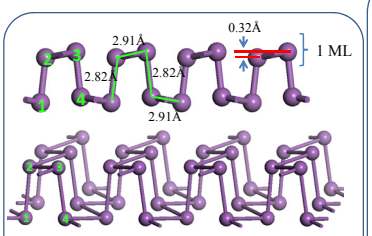


***E_e*(n)** : average extra energy of each atom in n ML Sb(110) compared with the energy in bulk. E_e(1) is extremely large.

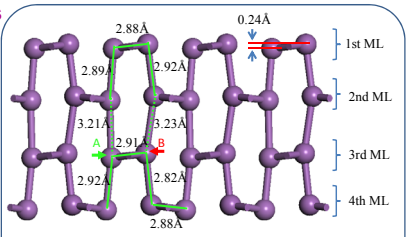
***E_d*(n)** = E_e(n)-(E_e(n-1)+E_e(n+1))/2, *i.e.*, E_d(n) is E_e(n) minus the average energy of E_e(n-1) and E_e(n+1).

If E_d(n) is much larger than 0, n ML is not stable, Since n layer thin film can always recompose to n-1 layer and n+1 layer to reduce the energy. 3 and 5 ML is not stable.

Ultrathin Sb (110) atomic structures

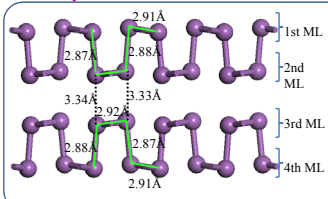


Side view (top) and perspective view (bottom) of **2 ML** Sb(110). Same atoms are indicated by the same numbers. Black phosphorus **(BP)-like structure.**



Side view of 4 ML Sb(110). Surface layer (1st and 4th ML) atoms are BP-like, different from non-surface layer atoms. Bonds between 1st and 2nd or 3rd and 4th ML is strong than that of between 2nd and 3rd ML. We call this as **BP-Bulk-like structure.** (similar structure for **≥ 4 ML** Sb(110))

Other possible structure?



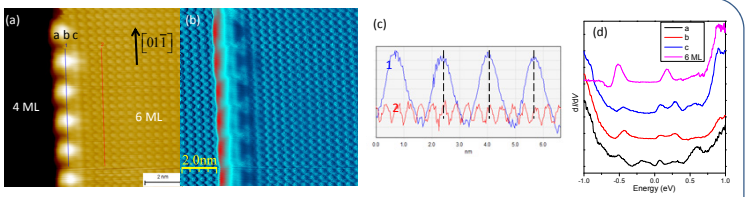
Commonly referred BP-like structure for 4 ML Bi(110)[2]. However, as **for the 4 ML Sb(110), Three evidences are for the BP-Bulk-like structure**:

(i) E_e are found to be 120.8 meV and 106.6 meV for the BP-like 4 ML model and BP-Bulk-like 4 ML model.

(ii) BP-Bulk-like structure can explain the odd-ML Sb(110) as well.

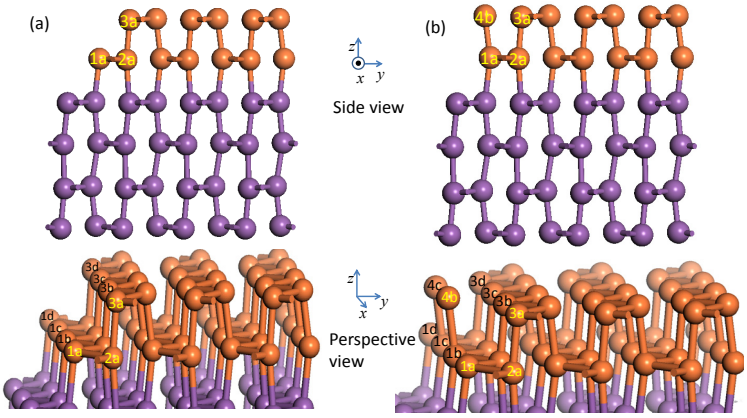
(iii) Calculated DOS (not shown here) from 4 ML BP-Bulk-like structure fit the STS better.

4 × 1 edge reconstruction



(a) Atomic-resolution STM image of the 4 × 1 edge reconstruction. Not all of the edges show reconstruction. (b) Derivative image of (a) to emphasize atomic resolution from two sides of the edge. (c) The blue line is the line profile extracted from panel (a) along the blue strait line. The red line is the line profile extracted from panel. (d) STS at three different points a, b and c, as indicated in panel (a), and STS on 6 ML Sb(110) far away from the edge. The edge states from point A are very localized.

Possible structures for the edge with and without reconstruction



(a) Edge without reconstruction. All atoms from the edge are saturated. (b) Edge with reconstruction. If by some chance, two atoms 4b and 4c connect to 1b and 1c, respectively. 4b and 4c connect to each other and they both connect to 3c to saturate dangling bonds. Repeating the unit cell in *x* direction leads to the 4 × 1 reconstruction.

4. Conclusions

- Below 6 ML, only even-ML Sb(110) islands form. Above 6 ML, both even- and odd-ML form. First-principles calculations support this growth mode.
- Ultrathin Sb (110) structure is relaxed.
- Some of the edges along $[01\bar{1}]$ show 4 × 1 reconstruction.

References

[1] G. Yao *et al., Sci. Rep.* ***3 (2013).***
[2] T. Nagao *et al., Physical Review Letters* ***93 (2004).***

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