

Growing quasi-freestanding phase germanene on Ag2Bi alloy Jang-Hung Yu, Chieh-Wei Peng

Advisor : professor Shu-Jung Tang

Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan

Abstract

In this work, we study the growth of germanene on Ag111 basis that depositing Bi atom. Bi will form three structures on Ag(111) according to different deposition amounts: Ag2Bi-Root3 X Root3 R30, Bi/Ag111-(p x root3), and Bi(110)/Ag(111). We use LEED(low energy electron diffraction) to investigate the germanene lattice structures formed by depositing Ge on two different Bi/Ag111 surfaces : **1**.Ag2Bi- $\sqrt{3}$ X $\sqrt{3}$ R30 alloy structure **2**.Coexistence structure of Ag2Bi- $\sqrt{3}$ X $\sqrt{3}$ R30 with Bi/Ag(111) - (p x $\sqrt{3}$)

- The first part, Ag2Bi alloy surface will de-alloy to Bi/Ag(111)-(p x $\sqrt{3}$) superstucture and qusai-freestanding phase germanene form side by side after depositing Ge. In addition, the pvalue decreases as the Ge deposition increases.
- The second part, also exhibits dealloying phenomenon, but the structure generated by Ge is SP germanene, with no observation of QP germanene formation. Moreover, the p-value is even smaller than that of the first part.

Using ARPES to measure the surface band structure and core-level variations in two distinct regions can be employed to compare with LEED results and draw conclusions. We finally constructed lattice models of the coexistence of Ag2Bi alloy - $\sqrt{3}$ X $\sqrt{3}$ R30 on Ag(111) - (p x $\sqrt{3}$) in order to explain the interesting structures observed in the second part of the experiments.

Theory

Depositing Bi on Ag 111strctrue:

According to the research by K.H.L Zhang [Ref.1], it is known that the deposition of Bi can result in various surface structures.



Figure 1 : (a) LEED data for Ag2Bi alloy- $\sqrt{3}$ X $\sqrt{3}$ R30 on Ag(111). (b) LEED data for Bi/Ag(111) -(p x $\sqrt{3}$) on Ag(111) .(c) LEED data for Bi(110) film on Ag(111) [Ref.1]

The dealloying process from Ag2Bi alloy to Bi/Ag(111) -(p x $\sqrt{3}$) involves a gradual transformation of the Bi atomic layers into a rectangular structure.



Figure 2 :

(a) Illustration of Bi atoms in real space on an Ag111 substrate. Gray represents Ag , green represents the upper layer of Bi atoms, and blue represents the lower layer of Bi atoms. The rectangle surrounded by black lines

The Corelevel and ARPES of Fig4 & Fig5 can be used to support our part1 results. In Fig5, we observed the emergy band structure of QP germanene.



Part2 : Depositing Ge on Bi/Ag(111)- $(p \times \sqrt{3})$ surface

In Part 2, we deposited Bi 120 min on Ag(111). Fig.6(a) can be observed that both the Ag2Bi alloy $\sqrt{3} \times \sqrt{3} \times \sqrt{3}$ R30 and (p x root3) scattering points appear simultaneously. Subsequently, Fig.6 (b to c) continuous deposition of Ge reveals that the p value gradually decreases with increasing Ge deposition. However, under part2 conditions, there are no diffraction points of QP germanene appearing near the diffraction points of $\sqrt{3}$ alloy. Instead, the angles of secondary diffraction points of Bi become smaller and gradually approach the diffraction point form of SP germanene.







represents the unit cell.

(b) Side and top view schematic diagram of the two-dimensional 2ML Bi(110) atomic structure, with the rectangular structure representing the unit cell. [Ref.2]

(p x $\sqrt{3}$) represents the lengths of a rectangle in two directions, where $\sqrt{3}$ denotes the vertical length and p denotes the horizontal length, with a value equal to the product of root3 and a variable. As the deposition of Bi increases, the value of p value decreases overall. When p value decreases to a certain extent, there will also be a certain compression in the $\sqrt{3}$ direction, making the structure more akin to a Bi(110) thin film structure.

Part1 : Depositing Ge on Ag2Bi/Ag(111)- $\sqrt{3} \times \sqrt{3}$ R30° alloy surface

First, Deposited Bi 60min on the Ag(111) substrate as shown in (Fig 3.a), where clear diffraction spots of Ag2Bi alloy - $\sqrt{3}$ X $\sqrt{3}$ R30 can be observed. Subsequently, increasing deposition of Ge (Fig 3.b to 3.d) reveals a gradual transition of Ag2Bi alloy $\sqrt{3}$ diffraction spots towards de-alloying process to form (p x $\sqrt{3}$) strctrue, where p decreases gradually. Simultaneously, diffraction spots of QP germanene appear outside the $\sqrt{3}$ alloy diffraction spots(Fig 3.Blue circle positon).



Figure 6 : (40ev) LEED data with simulation analysis for deposit (a) 120min Bi + 0min Ge (b) 120min Bi + 50min Ge(c) 120min Bi + 125min Ge

Through the ARPES results in Fig.7.(b), it can be observed that the energy band of SP germanene does appear, which proves that the LEED simulation results are correct. Therefore, we can infer that the rectangular structure of $(p \times \sqrt{3})$ will cause Ge atoms to prefer the growth of the Bi layer that continues the stripe arrangement to form SP germanene. Referring to the schematic diagram of Fig.9, the coexistence of the two structures on the substrate will further compress ($p \times \sqrt{3}$), making the p value smaller than part 1.





 $60\min Bi + 50\min Ge (d) 60\min Bi + 70\min Ge on Ag(111)$



Figure 4 : ARPES data use photon energy 30ev measure $\overline{\Gamma_{Aq}}$ to $\overline{M_{Aq}}$ of Ag₂Bi/Ag(111)- $\sqrt{3} \times \sqrt{3}R30^{\circ}$ alloy (a) +Ge 0min (b) Ge 25min(c) + Ge 50min

Figure 8 : The 80ev corelevel measured Bi deposit 120 min & according to the Ge depositing amount

photon energy 30ev measure $\overline{\Gamma_{Ag}}$ to $\overline{M_{Ag}}$ (upper) (a) Bi 120min + Ge 0min (b) Bi 120min + Ge 50min

Figure 9 : Schematic diagram of the dealloying process of Ag2Bi and SP germanene and

Summary

- Depositing Ge on Ag2Bi alloy surface induces the de-alloy process with the formation of QP germanene and Bi/Ag(111)-($p \times \sqrt{3}$). P value decreases from 0.924 $\times \sqrt{3}$ to 0.912 $\times\sqrt{3}$, when Ge coverage increases from 0.36 ML to 1 ML.
- Depositing Ge on Bi/Ag(111)- $(p \times \sqrt{3})$ surface induces the de-alloy process with the formation of SP germanene and Bi/Ag(111)-($p \times \sqrt{3}$). P value decreases from 0.925 $\times \sqrt{3}$ to 0.887 $\times \sqrt{3}$, when Ge coverage increases from 0.36 ML to 1.78 ML.
- A When the coverage of Ge increases on Bi/Ag(111)- $(p \times \sqrt{3})$, Bi/Ag(111)- $(p \times \sqrt{3})$ structure tend to be similar to SP germanene; in stripe direction, both lattice lengths are $\sqrt{3}$ and in armchair direction, p value of Bi/Ag(111)-($p \times \sqrt{3}$) decreases to get its lattice constant close to that of SP germanene.
- Photoemission measurement of valence energy band structure and core level states confirm the result of LEED measurement.

Reference

1. K H L Zhang et al 2012 J. Phys.: Condens. Matter 24 435502 2. Nano Lett. 2015, 15, 1, 80–87