# Growth of lead and gold layers on top of new quasi-freestanfing phase germanene

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## Abstract

Using low-energy electron diffraction (LEED) and angle-resolved photoemission spectroscopy (ARPES) techniques, we studied germanene on Ag(111) and divided our results into three parts:

1. At higher annealing temperatures, two new quasi-freestanding phases (QP) germanene, referred to as new QP1 and new QP2, were grown and compared with the QP R30° prevoously discovered.
2. Growth of two different monolayer Pb layers on the two new QP phases.
3. Au atoms infiltrate the Pb layer to form a special Au layer on new QP1 with the same lattice constant, 3.5Å, of the Pb layer, rather than the pristine one, 2.89Å.

## Effect of annealing temperature on QP germanene

Research from T.Y. Chen[1] found that on Ag(111) single crystal substrate, several different structures will be produced depending on the amount of Ge deposit. This poster focus on Quasi-freestanding Phase(QP).

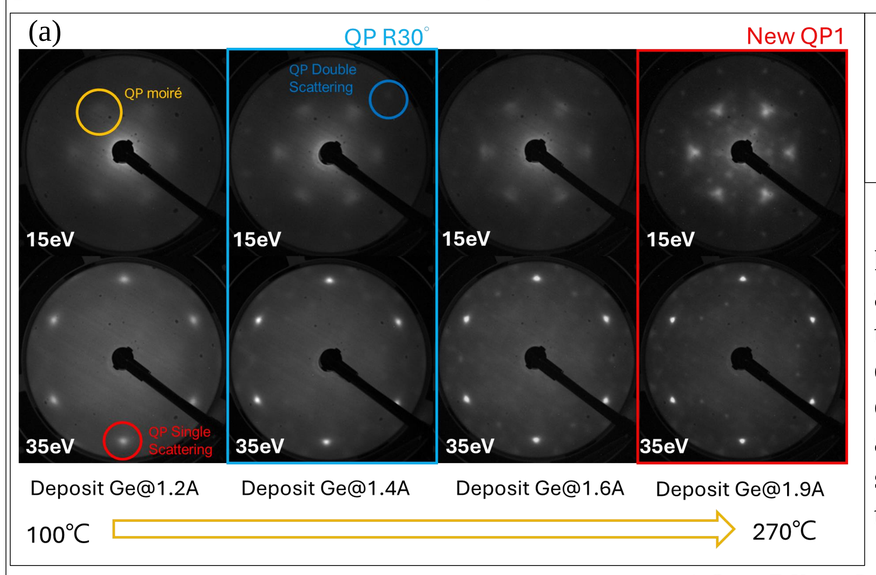
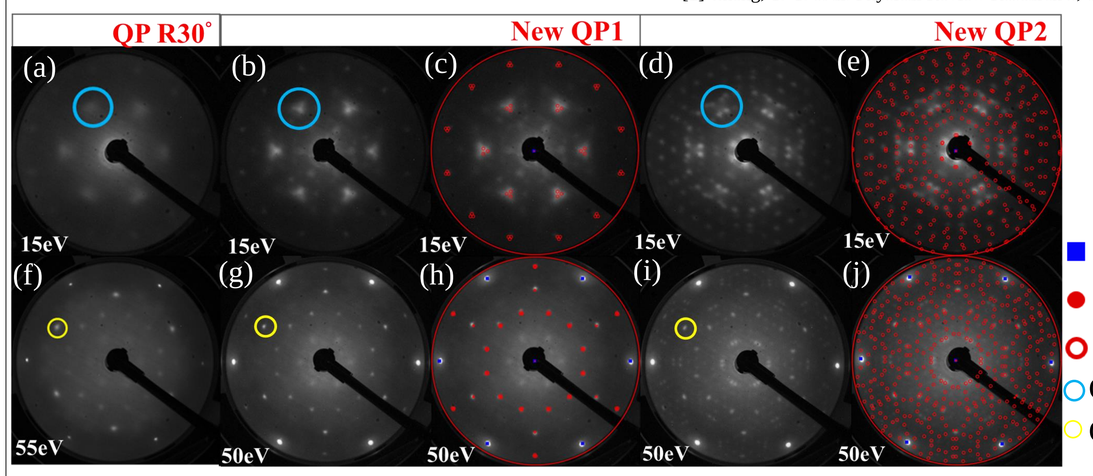



Fig.1(a) Due to the annealing temperature and the different amounts of deposited Ge atoms, observed that the primary and secondary diffraction spots are different from the original QP R30°.

[1] Cheng, T.-Y. et al. Physical Review Research 3, 033138(2021).




| Phase | a(Å) | γ | Coverage | Strain(%) |
|---|---|---|---|---|
| QP R30° | 3.91 | 60° | 1.08 | -3.7 |
| New QP Phase1 | 3.870 | 61.12° | 1.102 | -4.67 |
| New QP Phase2 | 3.968 | 60° | 1.06 | -2.27 |

Fig.2 The original QP moiré(a) is relatively blurry, new QP1(b) show three points and new QP2(d) is split into multiple points. The QP primary(f) diffraction patterns of the three phases are presented Paste, triangle, ellipse separately, new QP1 has a similar structure with QP R30°. New QP1 is composed of three domains, and the shape is a rectangle, angle 120° between with each other, so you will see three points, while new QP2 has two domains.

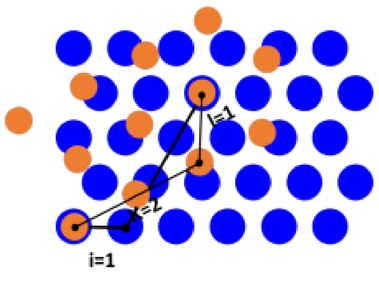
## High Order Coincidence

Higher-order coincidence (HOC) infers the lattice reconstruction between materials by calculating the recombination points between two layers of materials, including rotation angles and stresses on the materials.

So, for a hexagonal construction :

The lattice constants are a and b respectively, and the original vectors of the two layers of materials are vectors $(i, j)^T$ and $(k, l)^T$ respectively.

$$strain(\%) = \frac{\Delta_{kl}}{r_{kl}}, \qquad (\Delta_{kl} = r_{kl} - r_{ij}) \tag{1}$$




r is the length from the origin to the specified point, or calculated by referring to Löschian numbers

$$R(deg) = tan^{-1}\left(\frac{y_{kl}}{x_{kl}}\right) - tan^{-1}\left(\frac{y_{ij}}{x_{ij}}\right) \tag{2}$$

For the selected rotation angle of the substrate

$$density = \frac{1}{i^2 + ixj + k^2} \tag{3}$$

HOC density of upper material

## Table of Pb on new QP

| | Pb/New QP1 | Pb/New QP2 |
|---|---|---|
| Measurement angle | ±5.63 ° | ±5.285 ° |
| Simulation angle | ±5.685° | ±5.209° |
| QP strain | -4.377 % | 1.725 % |
| Pb strain | -3.272 % | -3.272 % |
| HOC density | 0.006 | 0.016 |
| Define coordinate | Ag(6, 10), QP(9, 3), Pb(10, 4) | Ag(9, 1), QP(4, 4), Pb(8, 0) |

The below table is the result after deposit Pb on two new QP, we use above equation to calculation strain, angle and density.

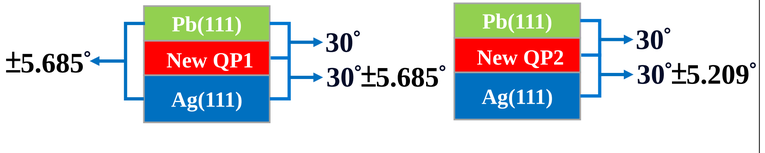



Table 1. Using i, j, k, l to calculate two different new QP effect.

## Grow Au layer on new QP1

We choose the new QP1 deposit Au.

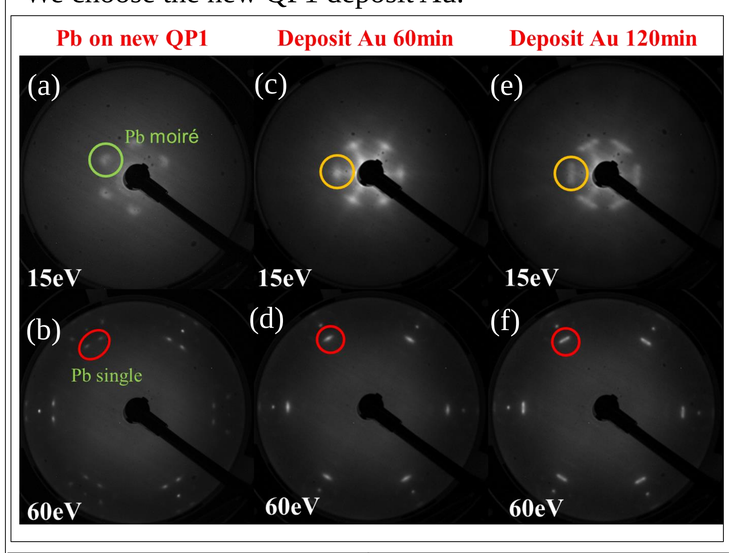



Fig. 3 LEED pattern of (a) & (b) are Pb on new QP1, (c) & (d) after deposit Au 60 mins to (a) & (b), (e)& (f) after deposit Au 120 mins to (c) & (d).

After deposit Au for 60min(c-d) & 120mins(e-f) respectively. (b) & (d) show that the primary diffraction point of Pb changed from a split point to a long strip . (d) & (f) show that the long strip pattern was composed of three points.

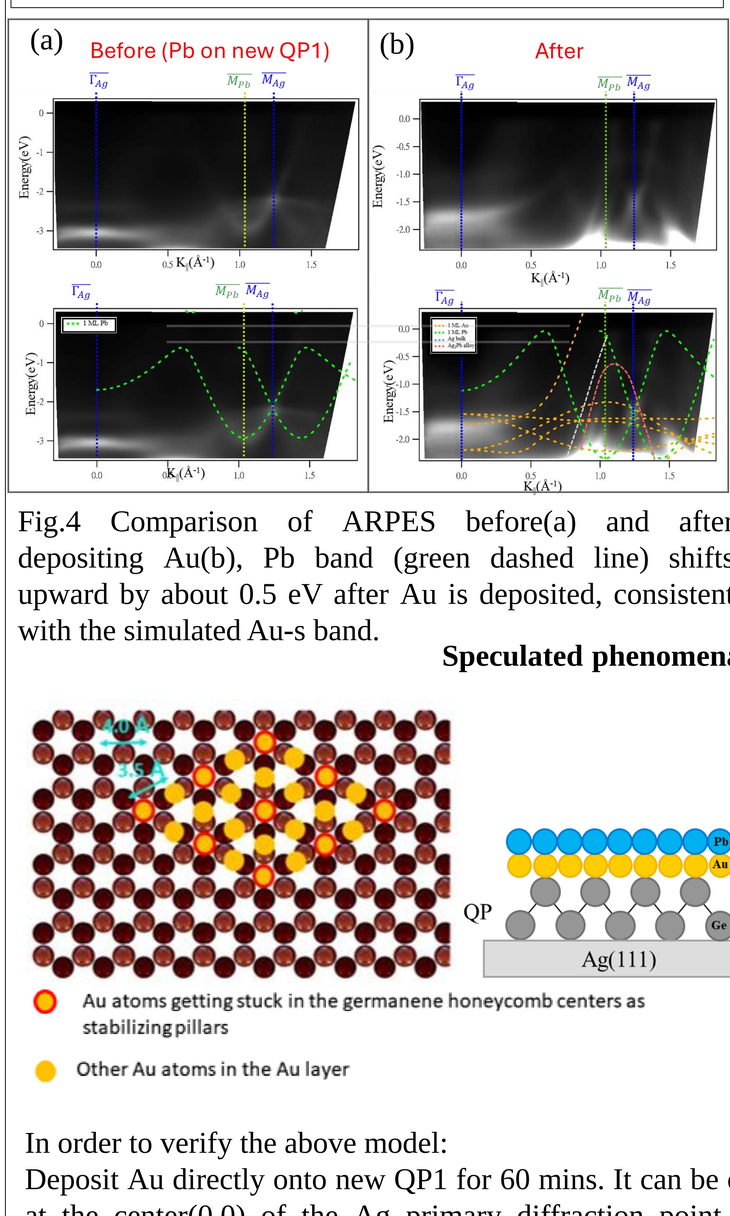



Fig.4 Comparison of ARPES before(a) and after depositing Au(b), Pb band (green dashed line) shifts upward by about 0.5 eV after Au is deposited, consistent with the simulated Au-s band.

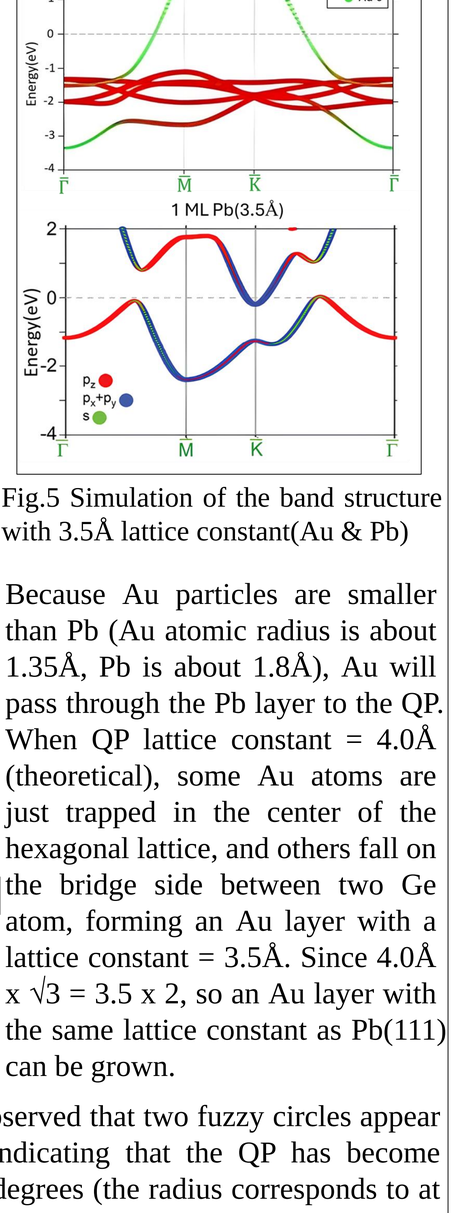



Fig.5 Simulation of the band structure with 3.5Å lattice constant(Au & Pb)

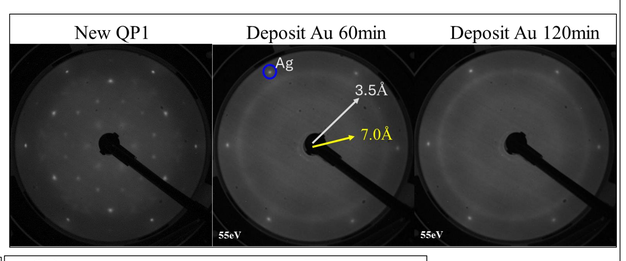



**Speculated phenomena:** Because Au particles are smaller than Pb (Au atomic radius is about 1.35Å, Pb is about 1.8Å), Au will pass through the Pb layer to the QP. When QP lattice constant = 4.0Å (theoretical), some Au atoms are just trapped in the center of the hexagonal lattice, and others fall on the bridge side between two Ge atom, forming an Au layer with a lattice constant = 3.5Å. Since 4.0Å x √3 = 3.5 x 2, so an Au layer with the same lattice constant as Pb(111) can be grown.

In order to verify the above model:

Deposit Au directly onto new QP1 for 60 mins. It can be observed that two fuzzy circles appear at the center(0,0) of the Ag primary diffraction point, indicating that the QP has become disordered and the domain exists in every direction in 360 degrees (the radius corresponds to at distances of 3.5Å and 7.0Å)

Fig.6 After depositing for another 60 mins, only some Au atoms are stuck in the center of the honeycomb, so the Au lattice constant in these areas = 7.0Å, and there are more Au atoms in some areas, inserted in the bridge side between the two hexagonal lattice (Au lattice constant= 3.5Å)



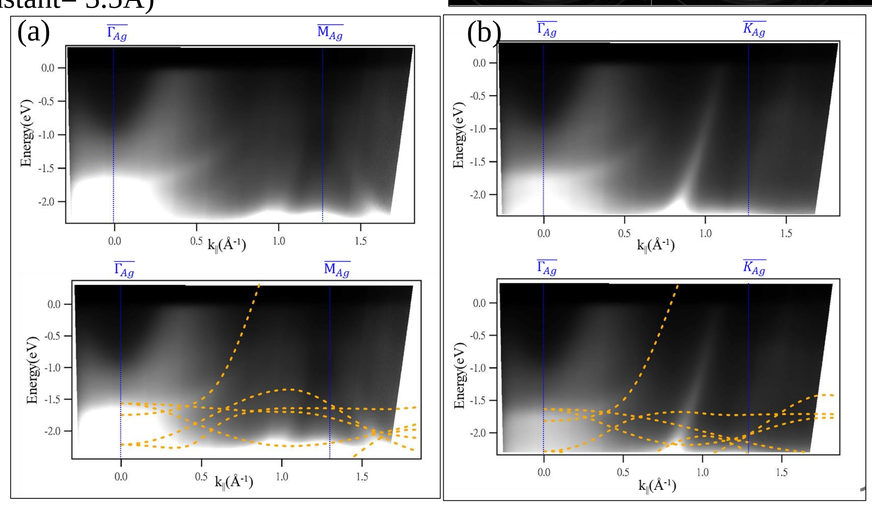




Fig.7 Energy band of deposited Au on new QP1
(a)direction is $\overline{\Gamma_{Ag}}$ to $\overline{M_{Ag}}$ of Ag(111)
(b)direction is $\overline{\Gamma_{Ag}}$ to $\overline{K_{Ag}}$ of Ag(111)

Overlay the simulation data and ARPES data, observe that Au-s energy band is consistent with the experiment, it mean that the Au on Pb on new QP1 is order, but we can't see the LEED spot form that result, our model explain that the Au LEED spot is overlay with QP spot, so the result support the hypothetical model.

## Summary

- Two new germanene phases obtained using higher annealing temperatures and analyzing LEED data through simulations.
- Deposit Pb on two new germanene phases, and calculate the strain, density and simulate angle of Pb in germanene/Ag(111) as mention above.
- Choose new QP1 to deposit Pb and then deposit Au, overlap the ARPES data with theoretically calculated energy band structure diagram to obtain a matching result.