# Study of PbAu alloy on different substrates

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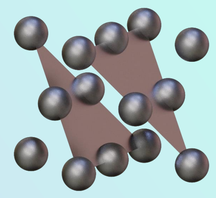


## Abstract


- When the system have time-reversal symmetry and inversion symmetry, the energy band of the system is not allowed to split. When one of the symmetries is breaking, the energy band is allowed to split.
- The model of PbAu alloy has a special configuration that induce inversion symmetry breaking then Rashba effect.
- Even under the same substrate, Different growth methods will also produce different rotation angles of alloy with substrate.


## Theory

Review:

### Time reversal symmetry

Time reversal $\hat{\theta}$ : When the system during time reversal($t \to -t$), its property(variables of physics) will stay the same or not.

$$\hat{\theta}\psi(r,t) = \psi^*(r,-t)$$

Kramers degeneracy theorem :

For every energy eigenstate of a time-reversal symmetric system with half-integer total spin, there is at least one more eigenstate with the same energy.

$$E(k,s) = E(-k,-s)$$

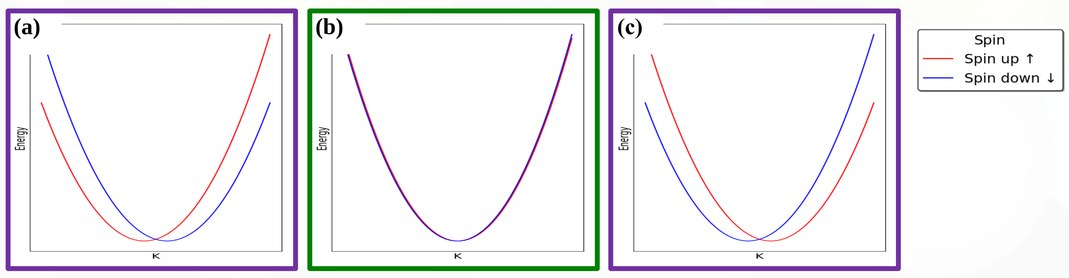



Fig 1.(a), (b), (c). All possible energy band of System with only time reversal symmetry

### Inversion(Parity) symmetry

Inversion $\hat{P}$: Inversion operate mean flip the sign of one or all spatial coordinate

$$\hat{P}: \begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} x \\ y \\ -z \end{pmatrix} \text{ or } \hat{P}: \begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} -x \\ -y \\ -z \end{pmatrix}$$

If a potential of crystal show property of inversion symmetry, it mean

$$E(k,s) = E(-k,s)$$

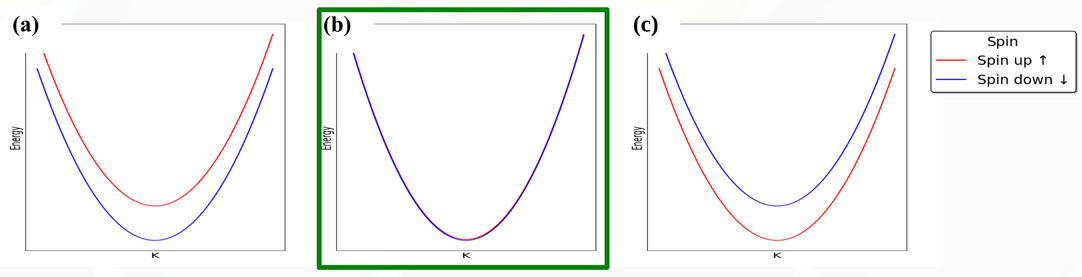



Fig 2.(a), (b), (c). All possible energy band of System with only inversion symmetry

Time reversal symmetry & Inversion symmetry

When combine time reversal symmetry and inversion symmetry, we can have

1. $E(k,s) = E(-k,-s)$
2. $E(k,s) = E(-k,s)$

$\Big\}$ $1 + 2 \Rightarrow E(k,s) = E(k,-s) \Rightarrow$ It satisfies only Fig 1.b & Fig 2.b

Time reversal symmetry & Inversion symmetry breaking

when combine time reversal symmetry and inversion symmetry breaking, we have

1. $E(k,s) = E(-k,-s)$
2. $E(k,s) \neq E(-k,s)$

$\Big\}$ $\Rightarrow$ It satisfies only Fig 1.a & Fig 1.c

### Spin–orbit coupling(SOC)

Spin magnetic moment can be expressed by below equation.

$\mu_s = -\frac{e\vec{S}}{2m_e} g_s$ , where $\vec{S}$ is spin angular momentum, $g_s$ is spin-g factor, $m_e$ is mass of electron.

The effective magnetic field can be expressed by below equation.

$B_{eff} = \frac{1}{c^2}\vec{E} \times \vec{v} = \frac{1}{4\pi\varepsilon_0}\frac{e}{r^3}\frac{\vec{l}}{m_e c^2}$ , where $\vec{E}$ is electric field of electron, $\vec{l}$ is orbital angular momentum, $c$ is speed of light.

When applied external magnetic field to magnetic moment, The potential can be express by

$U = -\vec{\mu} \cdot \vec{B}$ , where $\vec{\mu}$ is magnetic moment, $\vec{B}$ is the external magnetic field.

From above three equation, we can obtain the potential produced by SOC,

$$U_{soc} = -\overrightarrow{\mu_s} \cdot \vec{B}_{eff} = g_s \frac{1}{2}\frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r^3}\frac{1}{m_e{}^2 c^2}\vec{l} \cdot \vec{S}$$

We can observe that SOC related to $\vec{l} \cdot \vec{S}$, if we perform time reversal on $\vec{l} \cdot \vec{S}$ term, it will not change, it mean that when the system has SOC, it is time-reversal symmetric.

$\hat{\theta}\vec{l} \cdot \vec{S}\hat{\theta}^{-1} = (-\vec{l}) \cdot (-\vec{S}) = \vec{l} \cdot \vec{S}$

## Reference

[1] Chen, Wei-Chuan *et al.*, New J. Phys., 17., 083015 (2015).

## Model

- Model [1] is divided into 3 parts, Top Au , PbAu alloy and Bottom Pb layers.

1. Bottom Pb layers is Pb(111) lattice.
2. PbAu alloy layer is hexagonal lattice with buckled and is composed of Au atoms and Pb atoms, the buckling height is 1.8Å. The middle Au atom in alloy layer is $(0.95\sqrt{3} \times 0.95\sqrt{3})\ R30°$ lattice corresponding to bottom Pb layers.
3. Top layer capping Au atoms is Kagome lattice with the Au atoms in the alloy layer as the center.

- The key point of this model is the top of alloy covered with Au atoms with Kagome lattice, causes **bending configuration** of alloy film and thus induces inversion symmetry breaking.

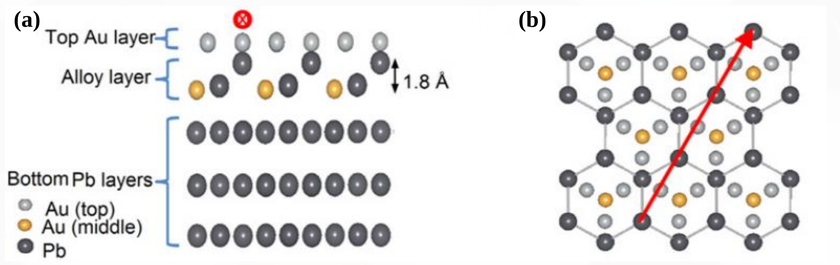
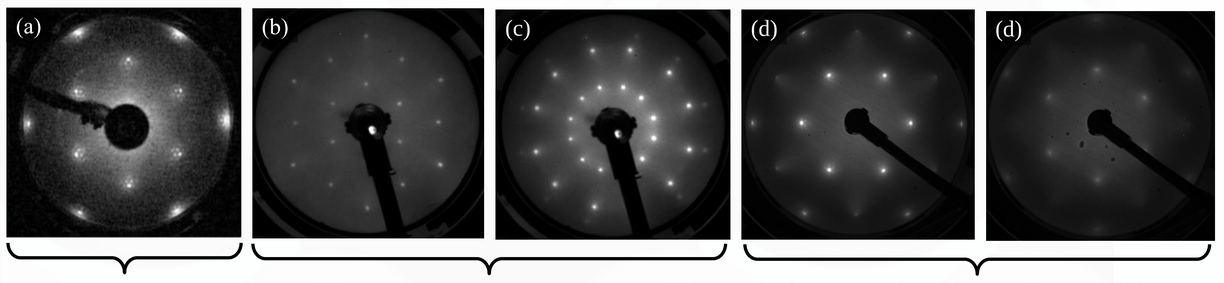



Fig 3. (a) Side view of PbAu alloy simulation model, the white/yellow/black sphere as Au(top)/Au(middle)/ Pb atoms. (b) Top view of (a).

## LEED

Fig 4




(a) PbAu alloy covered with a Au layer on bulk Pb(111) [1]

PbAu alloy with a Au layer on (b)1ML/(c) 2ML Pb film on bulk Ag(111)

PbAu alloy with a Au layer on (d)Thicker/ (e)Thinner wetting layer on bulk Ag(111)

- The LEED data(Fig 4.a-d) and its simulation(Fig 5.b) show PbAu alloy is $(0.95\sqrt{3} \times 0.95\sqrt{3})\ R30°$ lattice correspond to Pb layers.
- PbAu alloy can grown on Pb(111), Ag(111) and Ge(111) substrate, these PbAu alloy is the same lattice as mention before but rotate angle with substrate is difference.
- Under certain conditions, PbAu alloy can have different phases even on the same substrate.

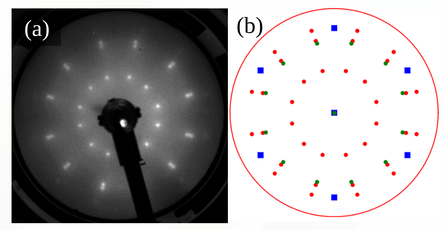



Fig 5.(a) PbAu alloy on 2ML Pb film, the angle of Pb film/PbAu alloy with substrate/Pb film is ± 13.9°/30°. (b) The LEED simulation of Fig5.(a), Blue/Green/Red spot as Ag(111), Pb & PbAu alloy.

## ARPES & PbAu alloy table

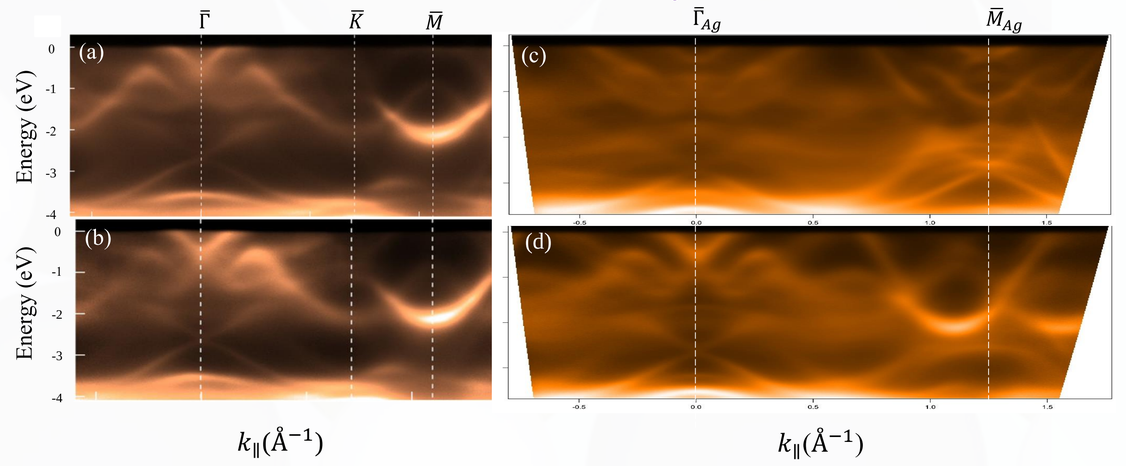



Fig 6. Energy band dispersion of PbAu alloy on (a) Pb(111) [1], (b) Ge(111) [1]. PbAu alloy on (c) 1ML Pb film (d) 2ML Pb film on Ag(111)

- The energy band structure of PbAu alloy have two cone-shaped band near surface zone center $\bar{\Gamma}$ at −0.56 eV & −2.65 eV. Rashba parameters is 1.53 & 4.45 eVÅ, the band structures of PbAu alloy grown on different substrates are similar.

| Substrate / Compare | Pb(111) (a) | Ag(111) (b) | Ag(111) (c) | Ge(111) (d) | Ge(111) (e) |
|---|---|---|---|---|---|
| Angle with substrate | 30° | 0° | 16.1° | 0° | 30° |
| Lattice constant | 5.7Å | 5.8Å | 5.8Å | 5.7Å | 5.7Å |
| Condition | Deposit Au at RT | Grown 1ML Pb film at LNT | Grown 2ML or above Pb film at LNT | Grown Thicker Au wetting layer | Grown Thinner Au wetting layer |

## Summary


- Time reversal symmetry & inversion breaking allow band splitting, the bending configuration of PbAu alloy cause the inversion symmetry breaking.
- LEED data show that lattice constant of PbAu alloy is around 5.7Å, it is $(0.95\sqrt{3} \times 0.95\sqrt{3})\ R30°$ lattice correspond to Pb layers. ARPES data show that energy band of PbAu alloys are almost the same, substrate do not affect construct of PbAu alloy.
- The other interesting thing that after form PbAu alloy, It forces the Pb layer to rotate 16.1° more, letting the angle between the Pb layer and Ag become 30°