# Rashba splitting in (111)-oriented PbSnTe:Bi topological crystalline insulator films

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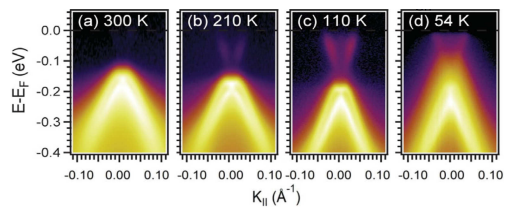
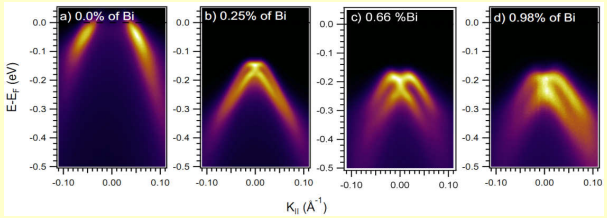
## Experiment




**Rashba effect** observed in ARPES maps of the MBE grown **$Pb_{0.54}Sn_{0.46}Te$ (111) epilayer topological crystalline insulator** (TCI) with Bi doping of 0.25% at.

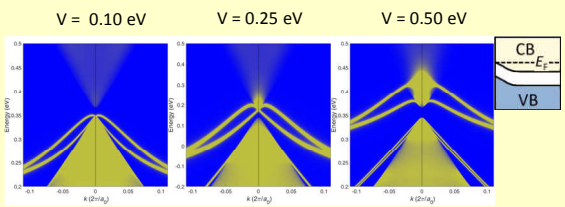
## Dependence on the Bi content - experiment



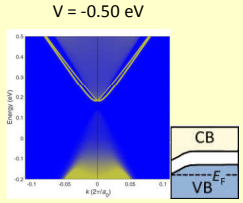

The increase of the Rashba splitting with increasing bulk Bi-doping indicates that surface charge is not constant but is controlled by the bulk Fermi level.

## Dependence on the Bi content (value of surface potential $V_0$)

T = 200K ; λ = 3 nm




$V_0$ positive ⇔ the charge $\sigma_S$ of the surface is negative and the bands bend upwards. The trap states have acceptor-like character.

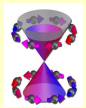



$V_0$ negative (positive $\sigma_S$, downward band bending) donor-like surface states.

## Topological insulators vs Rashba effect

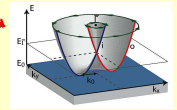
Topological Insulators (TIs) — Rashba effect

- Strong spin-orbit interactions
- Broken symmetry at the surface
- Helical states



Hamiltonian

$$H = b(k_x\sigma_y - k_y\sigma_x)$$

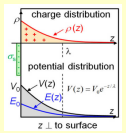


$b = \hbar v_F$, where $v_F$ is the Fermi velocity at the Dirac point.

$b$ is the Rashba parameter

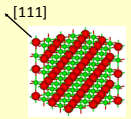
## Theoretical analysis

The presence of Bi atoms modifies the effective potential at the surface. This effect we simulated by applying the surface potential $V(z)$ according to Thomas-Fermi screening model with the initial value $V_0$ and screening length $\lambda$.




$$V(z) = V_0 e^{-z/\lambda}$$

We have analyzed (111) oriented $Pb_{1-x}Sn_xTe$ film with anion terminated surface. This material has:
- rock-salt crystal structure
- a narrow direct gap at 4 nonequivalent L-points.

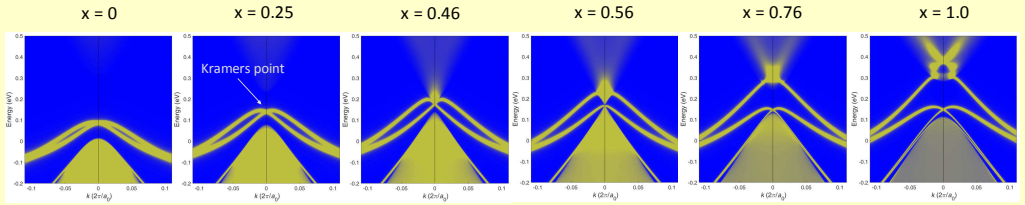



Using the tight-binding method we have calculated the surface spectral density of states.

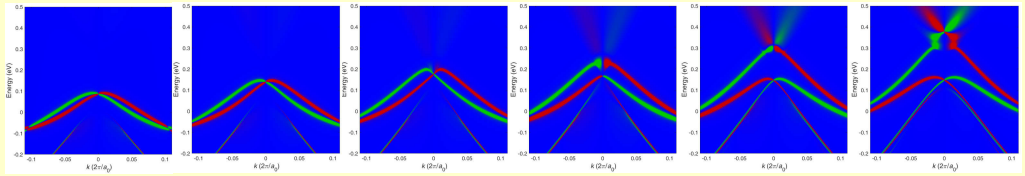
In the calculations we used $sp^3d^5$ parametrization with nearest neighbor and s-o interactions taken from C. Lent at al., Superlat. & Microstr. 2, 491 (1986).

## Dependence on the Sn content

T = 200K ; λ = 3 nm ; V = 0.25 eV



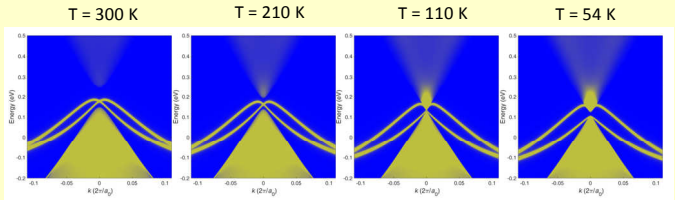

After the transition to TCI phase ($x_{Sn}$>0.37), the band above the Kramers point becomes the lower part of the Dirac cone and the band below the Kramers point forms the upper band of the new Rashba pair. The Dirac cone is highly deformed by Thomas Fermi potential, which shifts the Dirac point to the position, where it appears on the background of the conduction band.



Red (green) lines denote spin polarization perpendicular to Γ-K direction oriented into (out of) the figure plane. For TCI phase the spin chirality of the Rashba pair is opposite to the one in normal case, due to the band inversion.

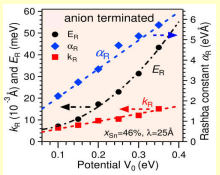
## Dependence on the temperature T

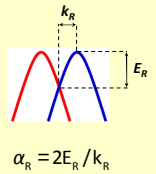
λ = 2.5 nm ; V = 0.20 eV




The gap closes at 110K. Below the band gap opens and the electronic band structure is inverted. Together with band gap also the gap in the Kramers point opens after decreasing the temperature.

## Dependence of Rashba parameters on the surface potential $V_0$




$$\alpha_R = 2E_R / k_R$$

The momentum splitting $\Delta k_R$ and Rashba constant $\alpha_R$ scale essentially linearly and $E_R$ squarely with increasing surface potential $V_0$.

## Conclusions

**Applied surface potential explains the Rashba splitting observed in (111)-oriented $Pb_{0.54}Sn_{0.46}Te$ films.**

**The increase of the Rashba splitting with increasing bulk Bi-doping indicates that surface charge is controlled by the bulk Fermi level.**

**RASHBA EFFECT COEXISTS WITH TCI PHASE in Bi-doped $Pb_{0.54}Sn_{0.46}Te$, BELOW 110K.**

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