SPIN STRUCTURE OF NON-MAGNETIC SURFACES BY ANGLE RESOLVED PHOTOEMISSION

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ES&ES, Kiev, 22/05/2013

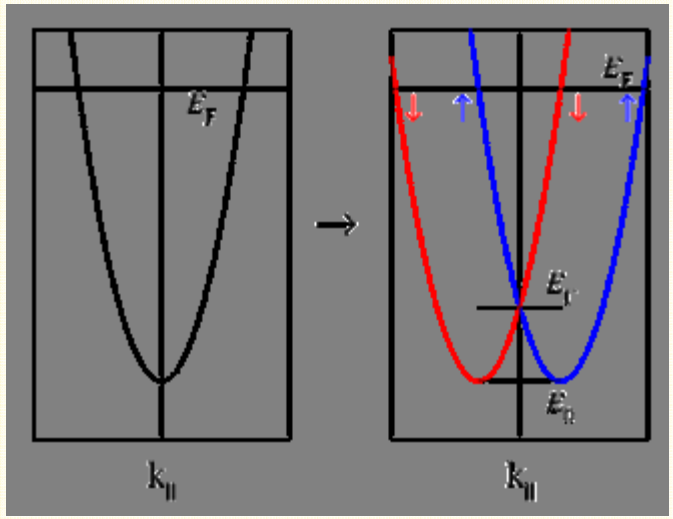
1. Origin of spin-polarization: Rashba effect

2. Rashba model and spin-orbit splitting in realistic crystals: role of in-plane scattering.

3. Rashba effect in bulk continuum.

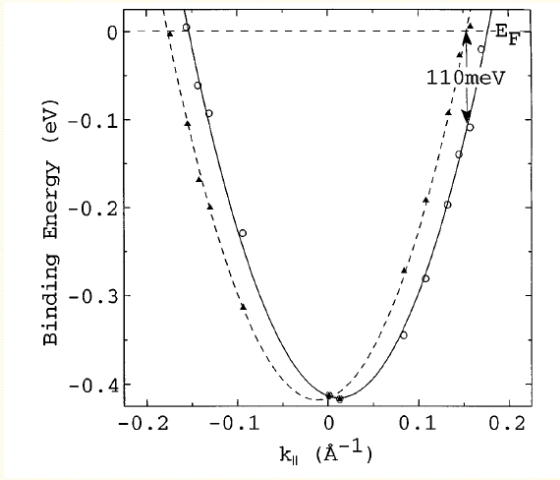
Effect of spin-orbit coupling on surface states: Rashba spin splitting

E.I. Rashba



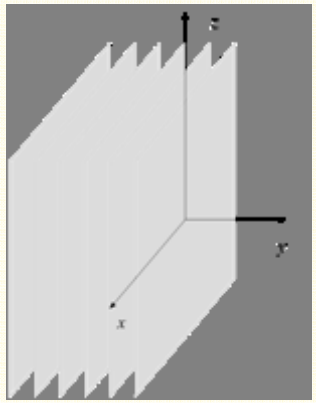
Rashba effect

E. I. Rashba and Yu. A. Bychkov, J. Phys. C **17** , 6039 (1984)



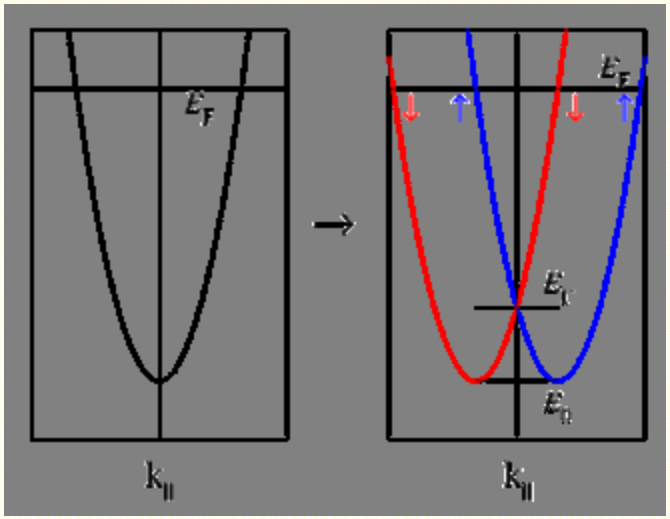
S. LaShell, B.A. McDougall, and E. Jensen, Phys. Rev. Lett. **77**, 3419 (1996)

Rashba model



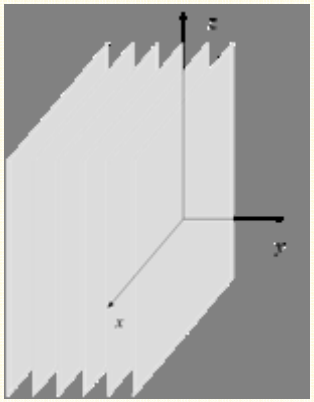
Rashba Hamiltonian $H_{\mathrm{R}} = \rho[\nabla V]\vec{\sigma} \cdot (\vec{k}_{||} \times \vec{e}_n)$

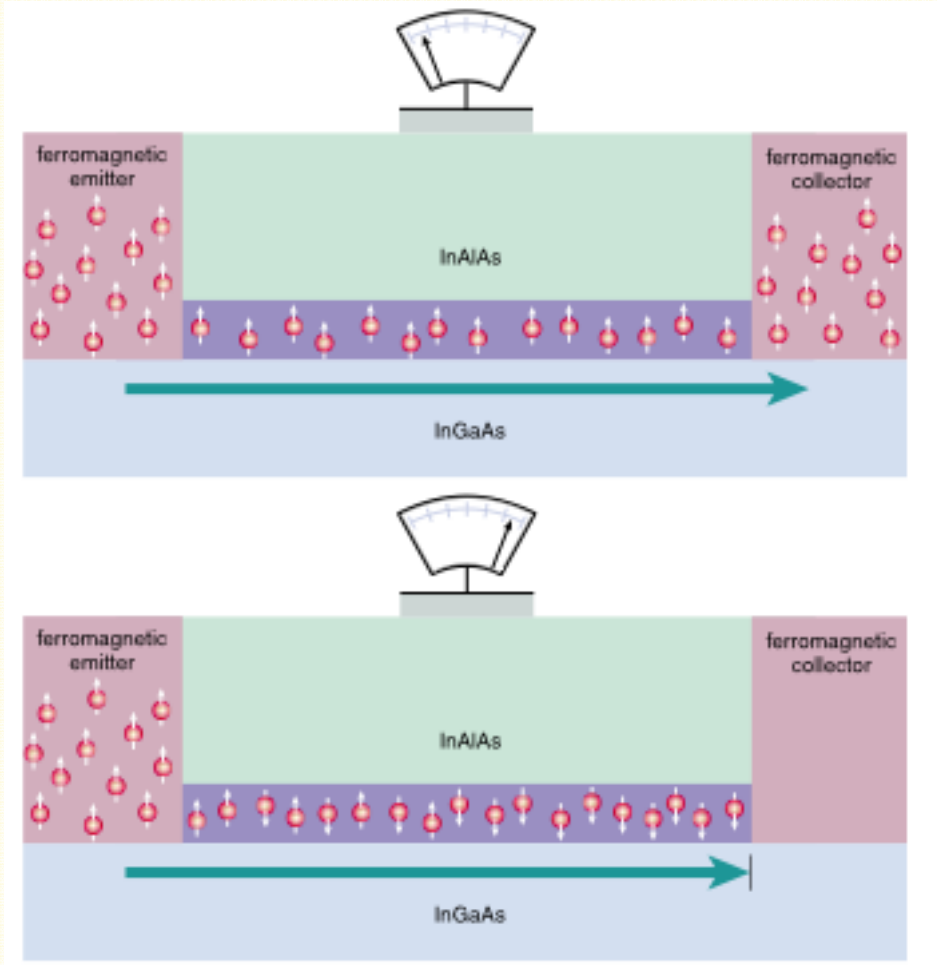
Datta-Das spin transistor



spin-dependent transport along *x*:

different $\mathbf{k}_{||}$ for the two spins ➔
phase shift at the collector

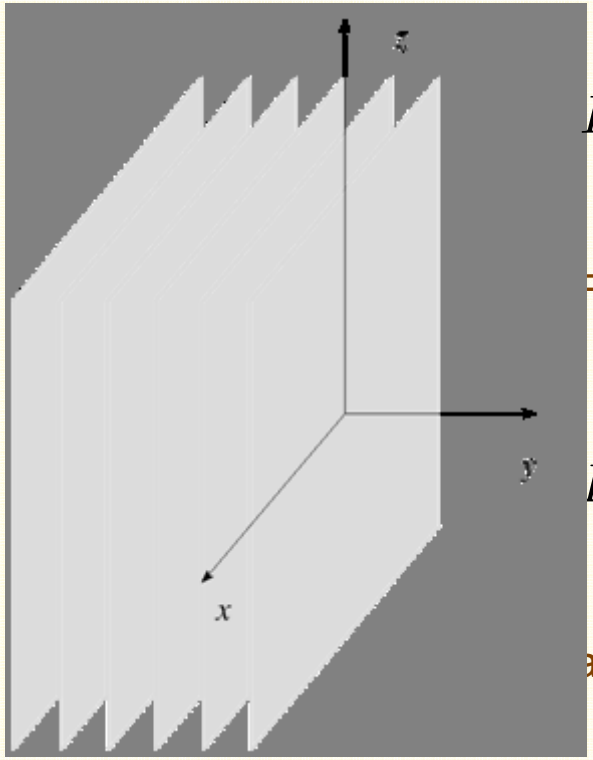




adapted from
Sankar Das Sarma, *American Scientist* **89**, 516 (2001)

Origin of the Rashba spin splitting: complex band structure view

Starting with the two-component Hamiltonian



$$\hat{H} = \frac{p^2}{2m} + V(\vec{r}) + \frac{\hbar}{4m^2c^2}\,\vec{\sigma}\cdot\left[\vec{\nabla}V(\vec{r})\times\vec{p}\right].$$

For a potential without lateral corrugation it reads

$$\hat{H} = \hat{H}_0 + \frac{\alpha^2}{4}\left[\begin{pmatrix} -V_y' & 0 \\ 0 & V_y' \end{pmatrix}\hat{p}_x + \begin{pmatrix} 0 & V_y' \\ V_y' & 0 \end{pmatrix}\hat{p}_z\right]$$

and for $k_{||}$ along x the equations for the two spin variables separate

$$\hat{H}_0\begin{pmatrix}\psi^{\uparrow}\\ \psi^{\downarrow}\end{pmatrix} + \eta\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix}\psi^{\uparrow}\\ \psi^{\downarrow}\end{pmatrix} = E\begin{pmatrix}\psi^{\uparrow}\\ \psi^{\downarrow}\end{pmatrix},$$

Origin of the Rashba spin splitting: complex band structure view

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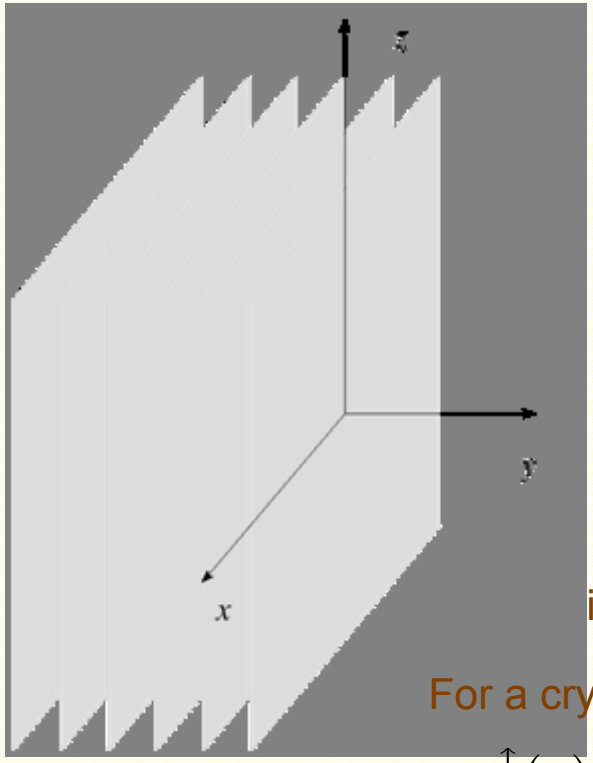


$$\hat{H}_0 \begin{pmatrix} \psi^{\uparrow} \\ \psi^{\downarrow} \end{pmatrix} + \eta \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \psi^{\uparrow} \\ \psi^{\downarrow} \end{pmatrix} = E \begin{pmatrix} \psi^{\uparrow} \\ \psi^{\downarrow} \end{pmatrix},$$

and the problem is reduced to a pair of scalar 1D equations

$$-\psi'' \pm \eta\psi + V\psi = (E - k_{||}^2)\psi \quad \text{where} \quad \eta = \frac{\alpha^2}{4} V_y' k_|$$

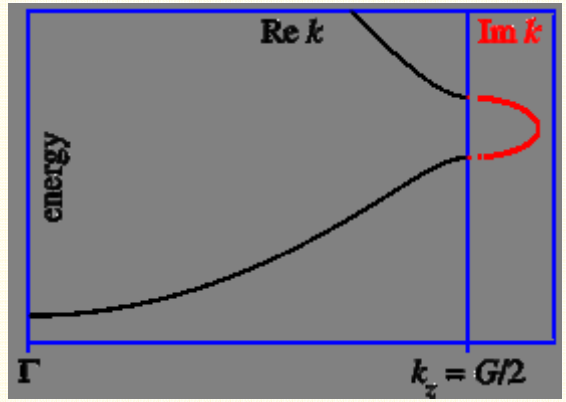
with the effective potentials $v^{\uparrow} = V + \eta$ and $v^{\downarrow} = V - \eta$

For a crystal with inversion $V(y) = V(-y)$

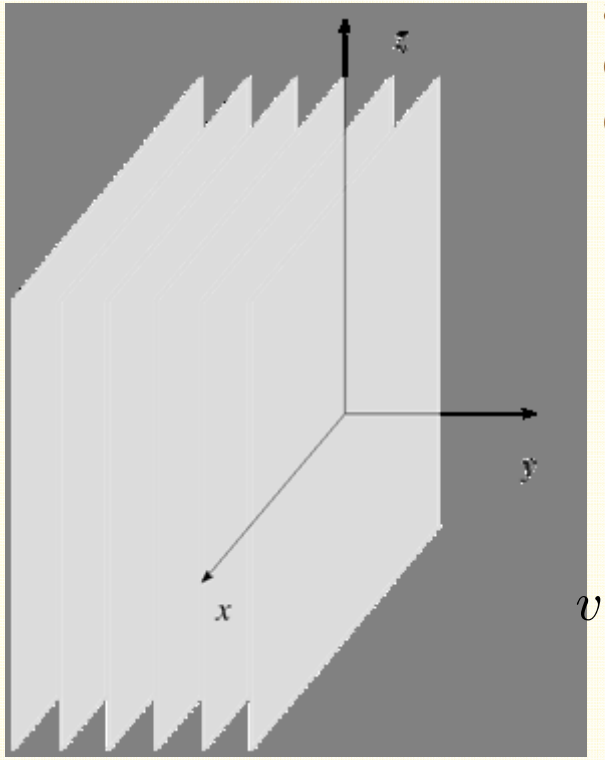
it is $v^{\uparrow}(y) = v^{\downarrow}(-y)$, so the two potentials

yield the same band structure,

and there is no splitting in the bulk.



Origin of the Rashba spin splitting: complex band structure view



In the Rashba model the relativistic spin split surface states arise as solutions of two decoupled scalar Schrödinger equations for the effective potentials for the two spins connected as $v^{\uparrow}(y) = v^{\downarrow}(-y)$

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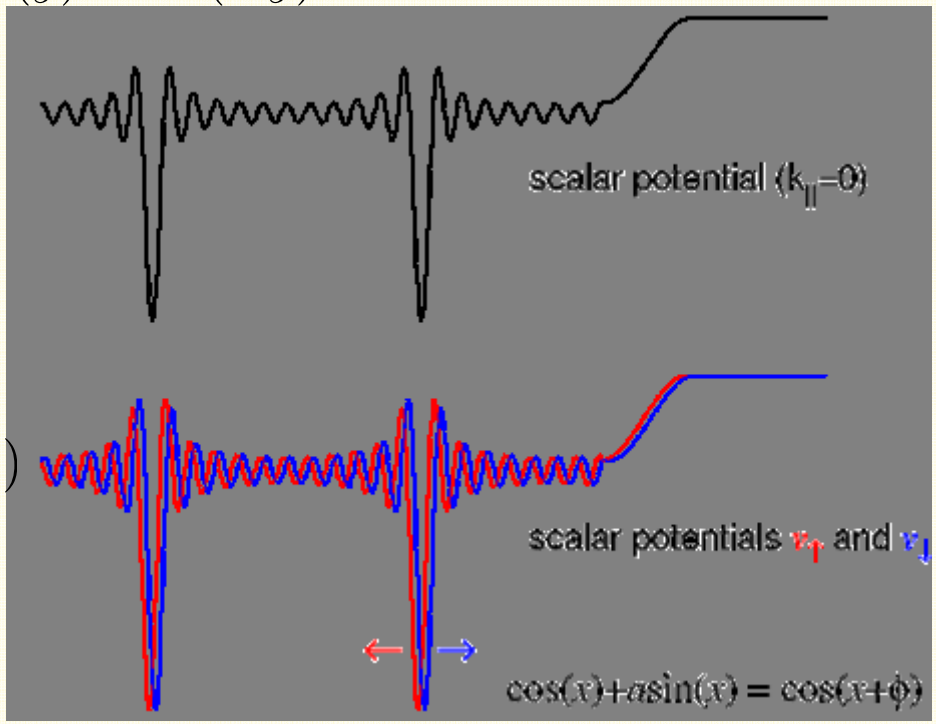
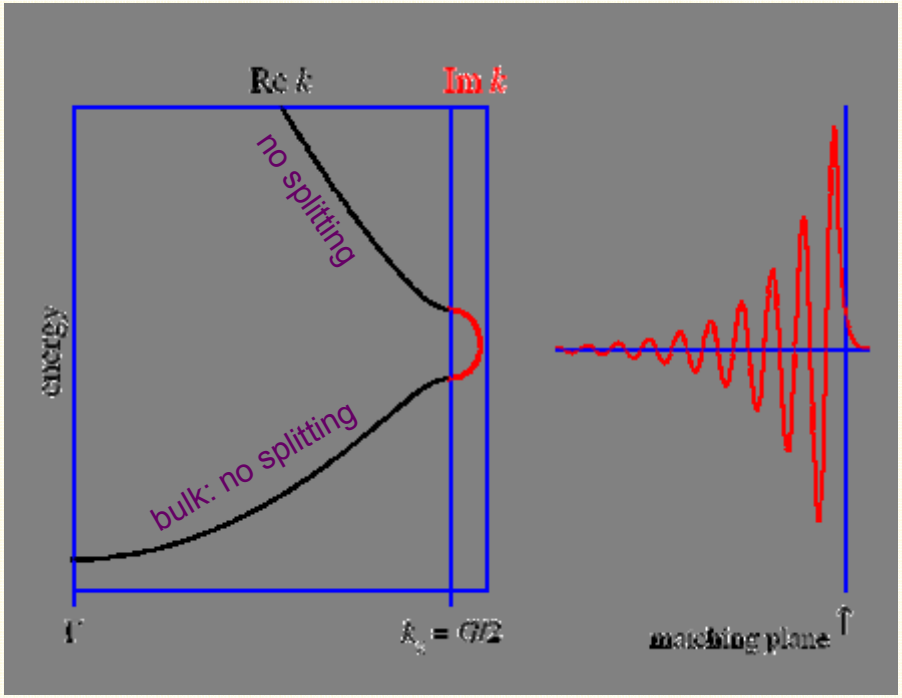


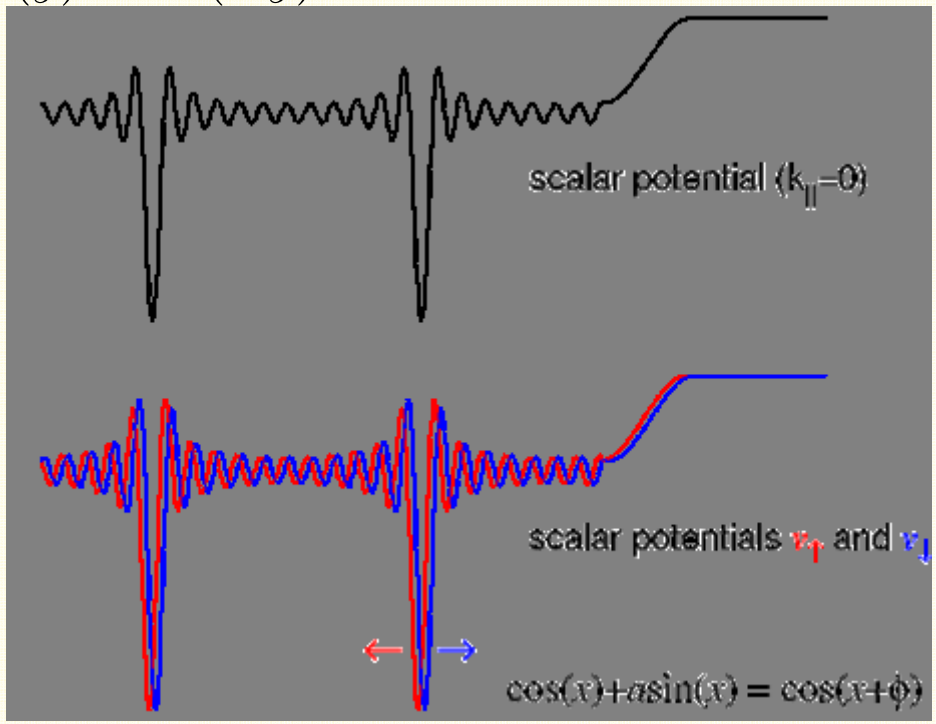
$V(y) = V(-y)$

The two (non-symmetric) potentials produce the same band structure (real and complex) but different wave functions → splittng of surface states.

Origin of the Rashba spin splitting: complex band structure view

In the Rashba model the relativistic spin split surface states arise as solutions of two decoupled scalar Schrödinger equations for the effective potentials for the two spins connected as $v^{\uparrow}(y) = v^{\downarrow}(-y)$



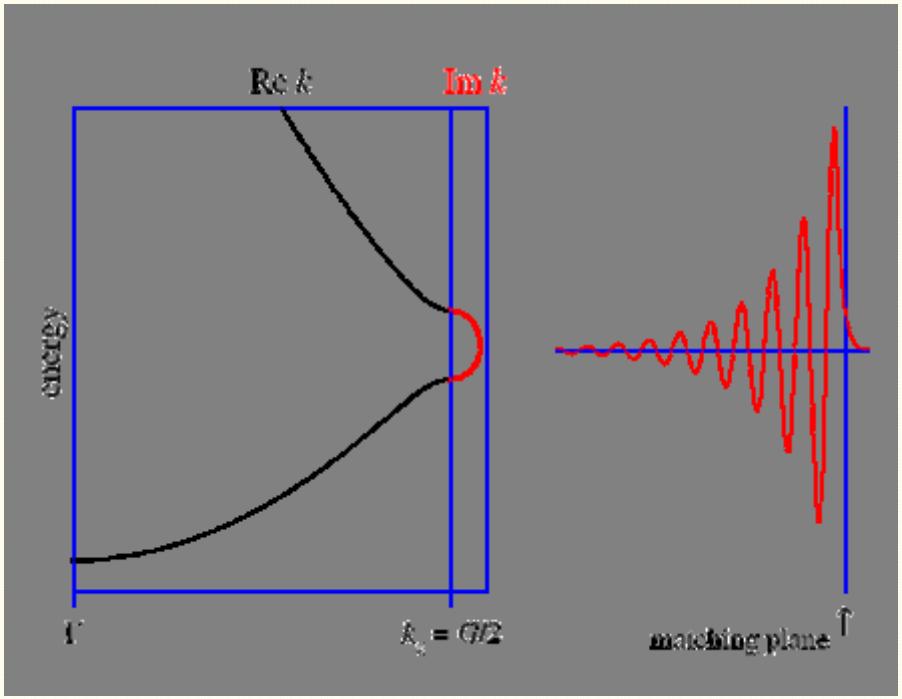


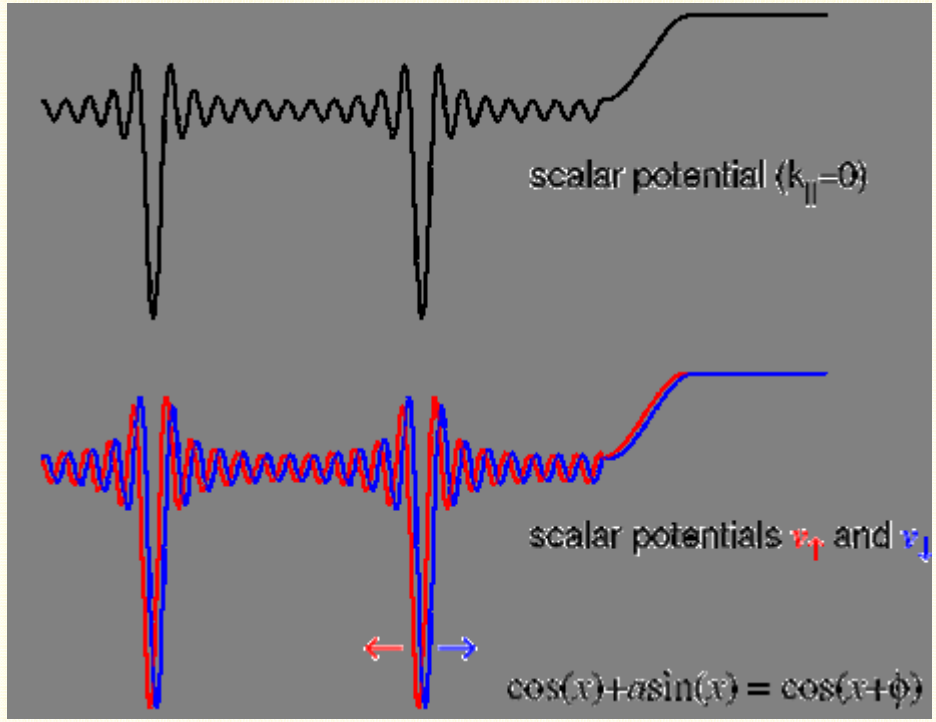
The two (non-symmetric) potentials produce the same band structure (real and complex) but different wave functions → splittng of surface states.

Origin of the Rashba spin splitting: complex band structure view

Rashba model:

- Exactly solvable minimal model to yield spin splitting.
- Potential gradients are too small at reasonable gaps.





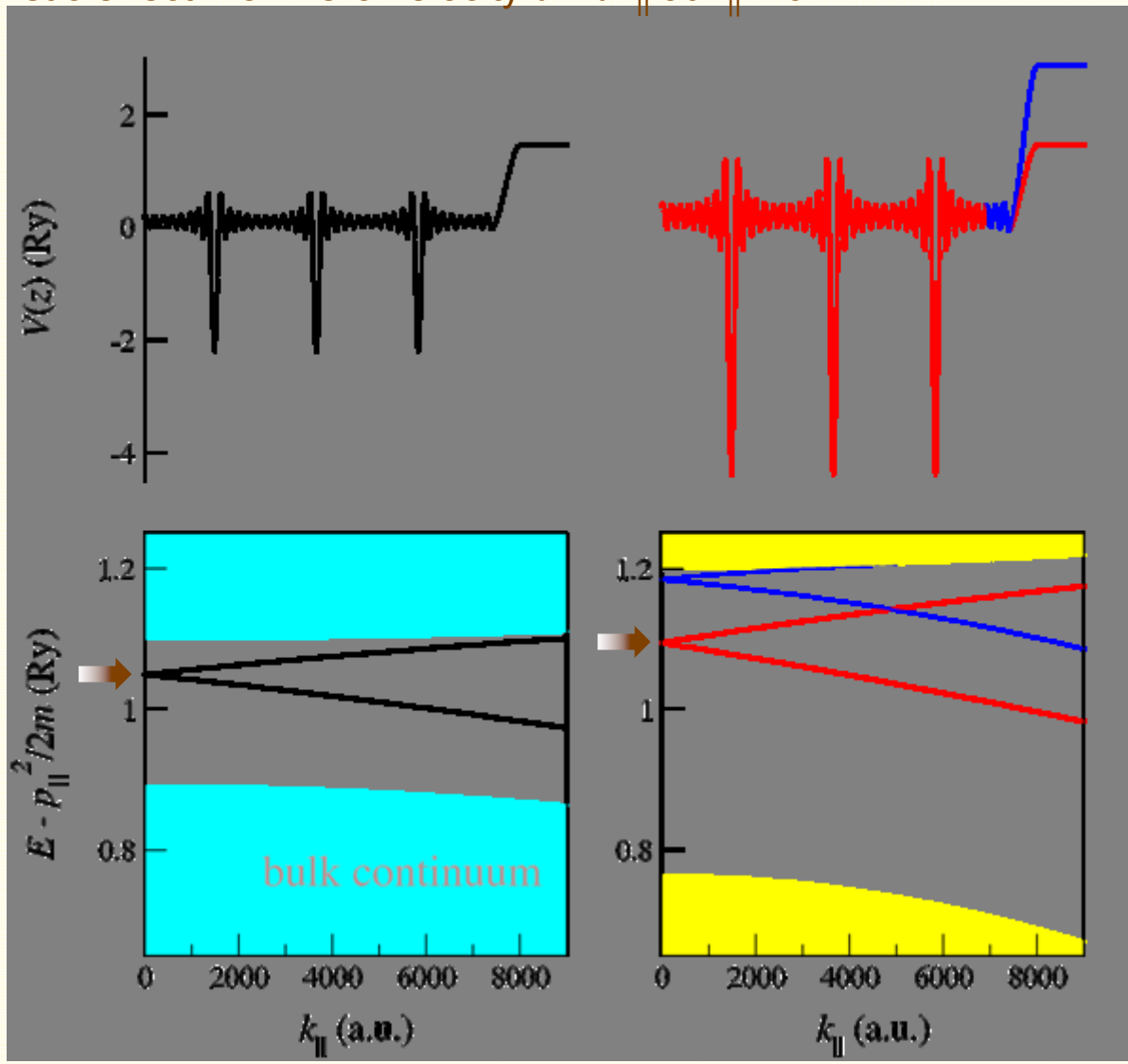
Rashba Hamiltonian $H_{\mathrm{R}} = \rho[\nabla V]\vec{\sigma} \cdot (\vec{k}_{||} \times \vec{e}_n)$

What determines the size of the spin splitting in the Rashba model?

The essence of the relativistic effect: non-zero velocity $dE/dk_{||}$ at $k_{||} = 0$.

Dependence of the surface state splitting on the crystal potential:

the size of the splitting is not simply related to the potential gradient.



What determines the size of the spin splitting in the Rashba model?

The essence of the relativistic effect: non-zero velocity $dE/dk_{||}$ at $k_{||} = 0$.

$$\left\{ \hat{H}_0 + 2\vec{k}\cdot\hat{\vec{p}} + k^2 + \frac{\alpha^2}{2}\,\vec{\sigma}\cdot\left[\vec{\nabla}V\times\vec{p}\right]\right\} \quad \Psi_0 \quad + \tag{1}$$

$$\frac{\alpha^2}{2}\,\vec{\sigma}\cdot\left[\vec{\nabla}V\times\vec{k}\right] \quad \Psi_0 \quad = E\,\Psi_0,$$

$$\text{where } \hat{H}_0 = \frac{\hat{p}^2}{2m} + V(\mathbf{r}) \text{ and } \Psi = \Psi_0 e^{i\mathbf{kr}} = \begin{pmatrix} \psi^{\uparrow} \\ \psi^{\downarrow} \end{pmatrix} e^{i\mathbf{kr}},$$

$$\frac{dE}{d\vec{k}} = 2\left\langle \Psi_0 \left| \hat{\vec{p}} \right| \Psi_0 \right\rangle + \frac{\alpha^2}{2}\left\langle \Psi_0 \left| \vec{\sigma}\cdot\left[\vec{\nabla}V\times\vec{\kappa}\right] \right| \Psi_0 \right\rangle, \tag{2}$$

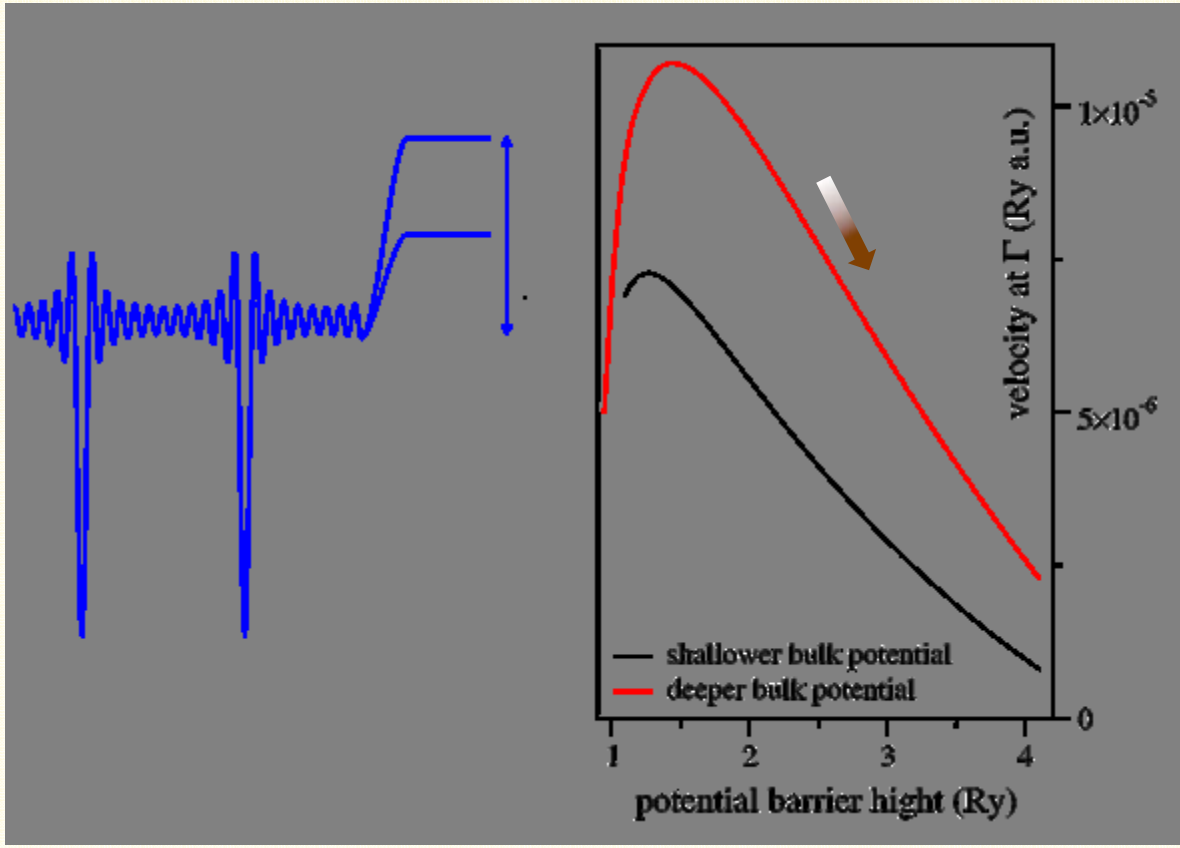
Velocity at $k_{||} = 0$ is the expectation value of the potential gradient.

What determines the size of the spin splitting in the Rashba model?

The essence of the relativistic effect: non-zero velocity $dE/dk_{||}$ at $k_{||} = 0$.

Dependence of the surface state splitting on the crystal potential barrier:

the size of the splitting diminishes with increasing the surface potential barrier.



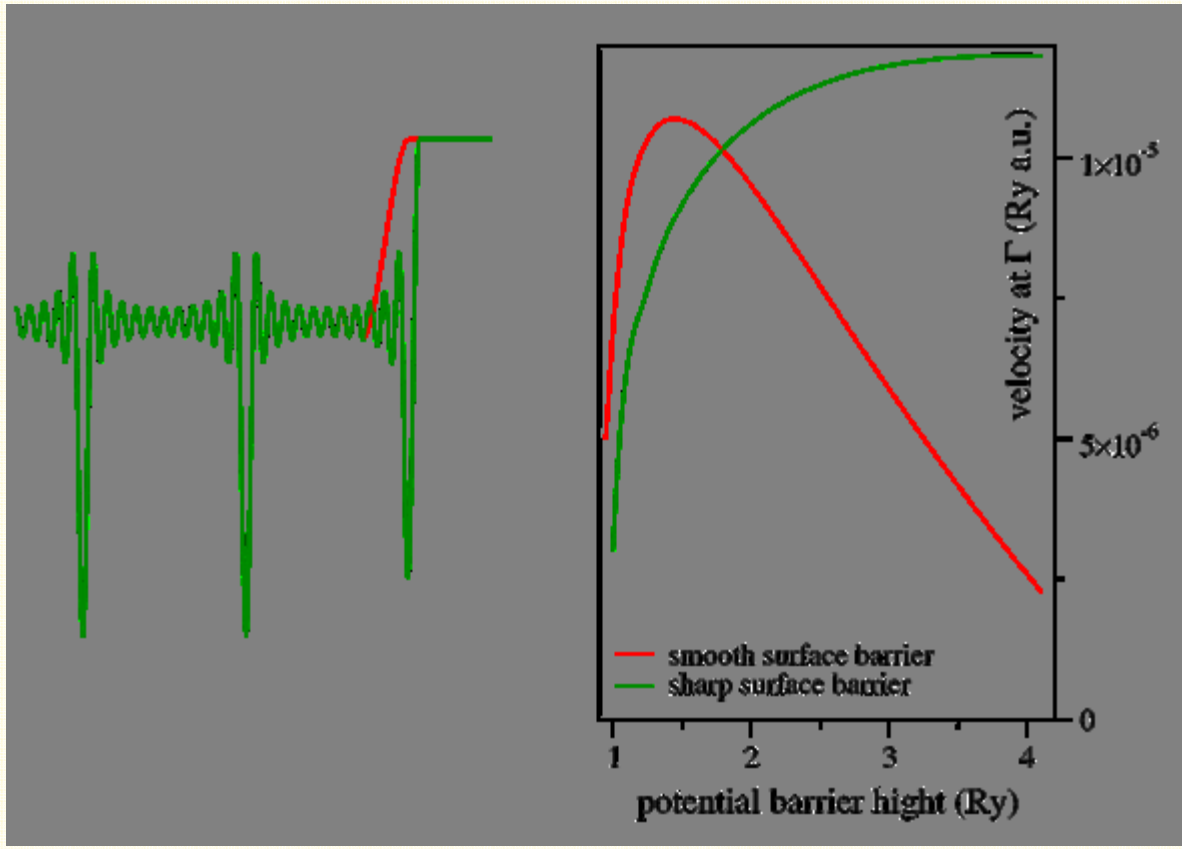
What determines the size of the spin splitting in the Rashba model?

The essence of the relativistic effect: non-zero velocity $dE/dk_{||}$ at $k_{||} = 0$.

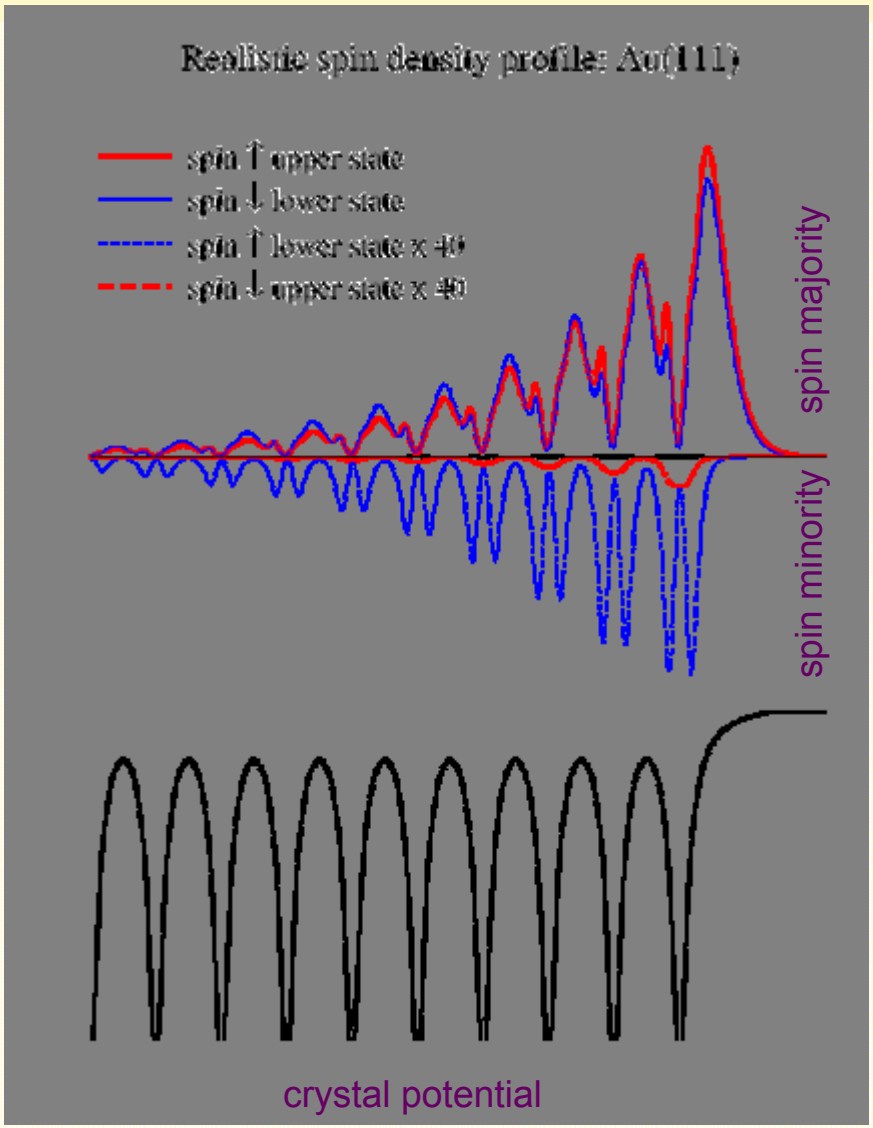
Dependence of the surface state splitting on the shape of crystal potential barrier.

The size of the splitting depends on the shape of the surface potential barrier in a complicated manner:

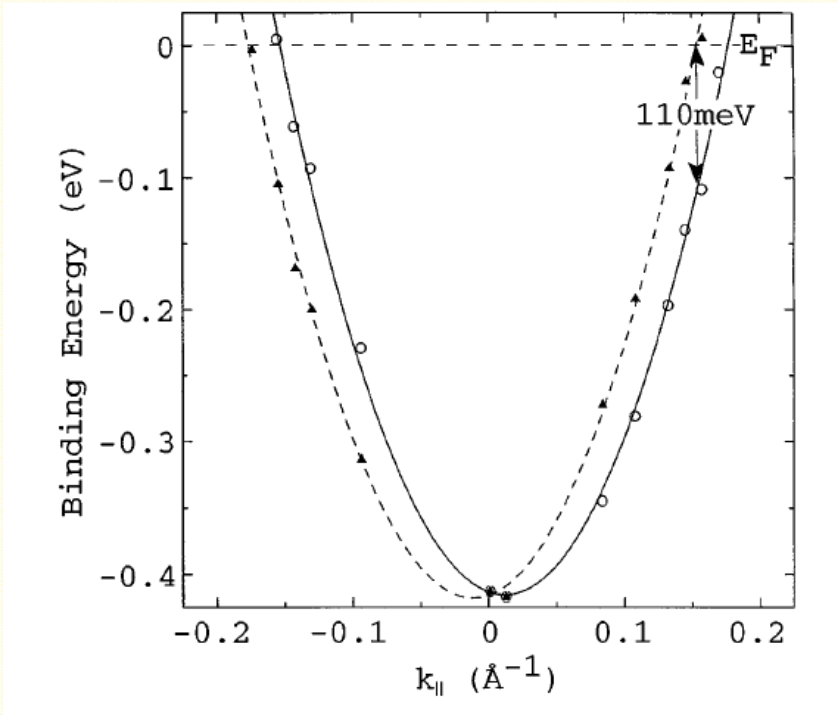
a singularity at the surface may increase or decrease the splitting.



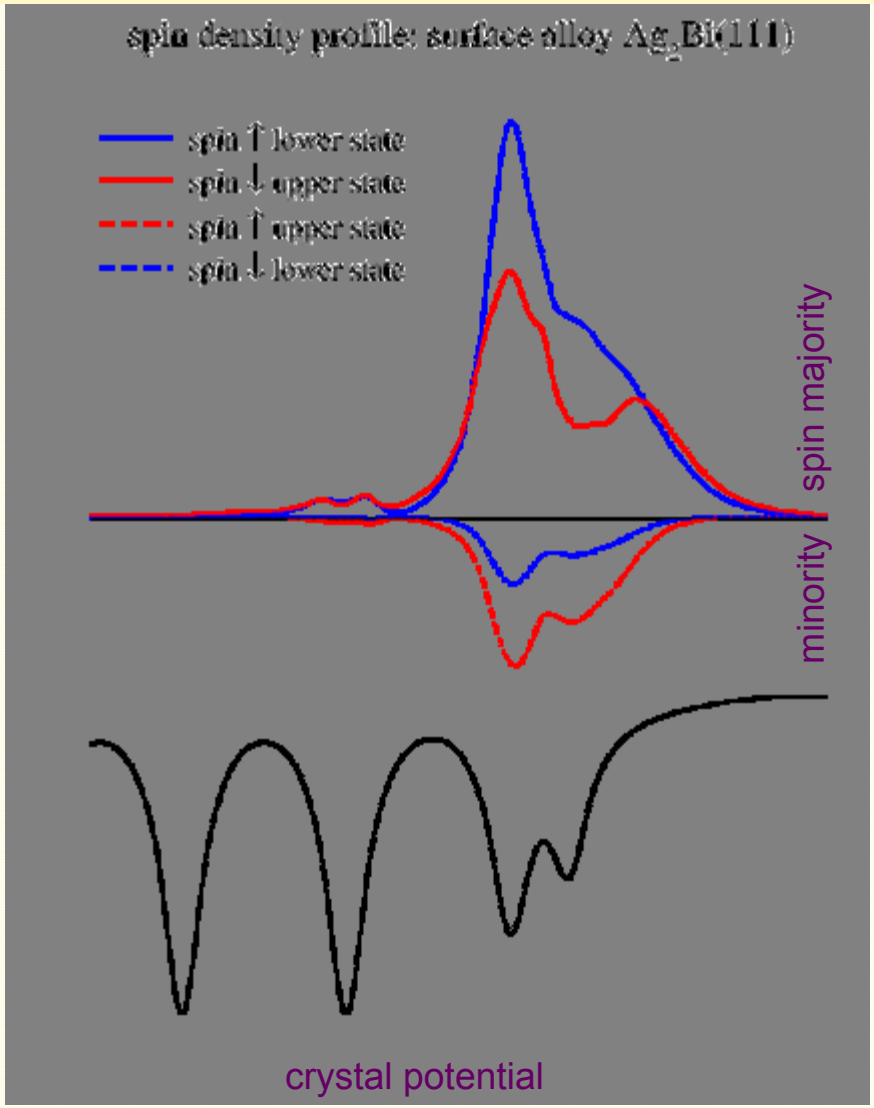
Rashba splitting at realistic surfaces: Au(111)



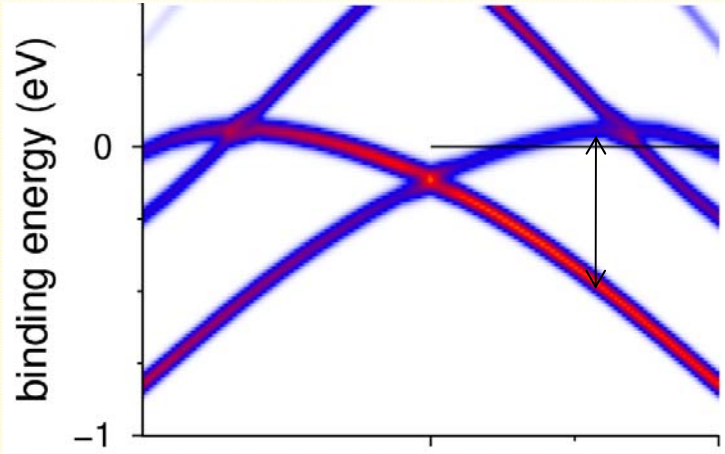
1. Energy splitting is about 0.1 eV.
2. Decay factors for the two states are slightly different.
3. Spin polarization is ~ 100% (although it is slightly different).



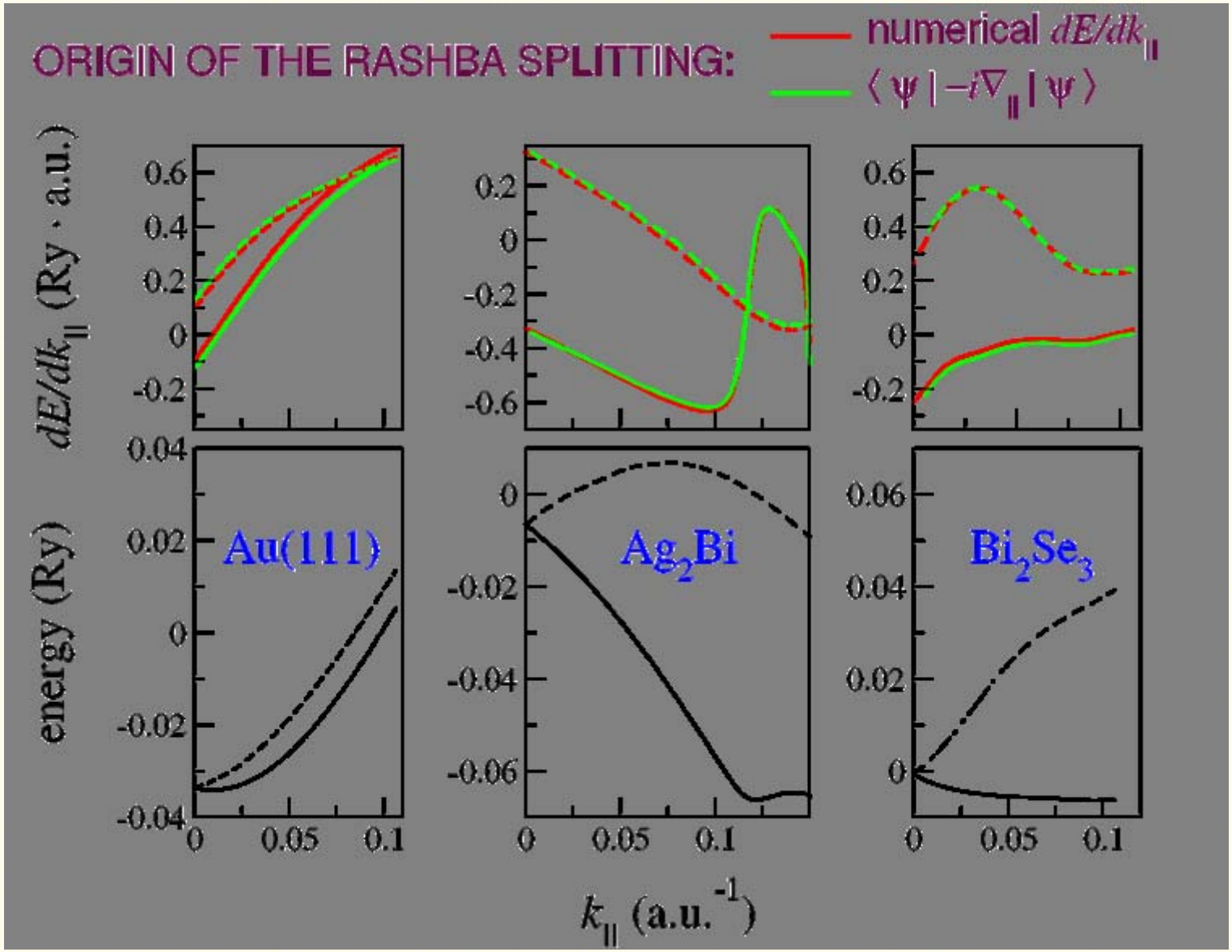
Rashba splitting at realistic surfaces: Ag_2Bi



1. Energy splitting is about 0.5 eV.
2. The states are strongly localized at the outermost layer.
3. Spin polarization is much less than 100%, and it is strongly different.



Spin splitting at realistic surfaces depends on the non-relativistic term.

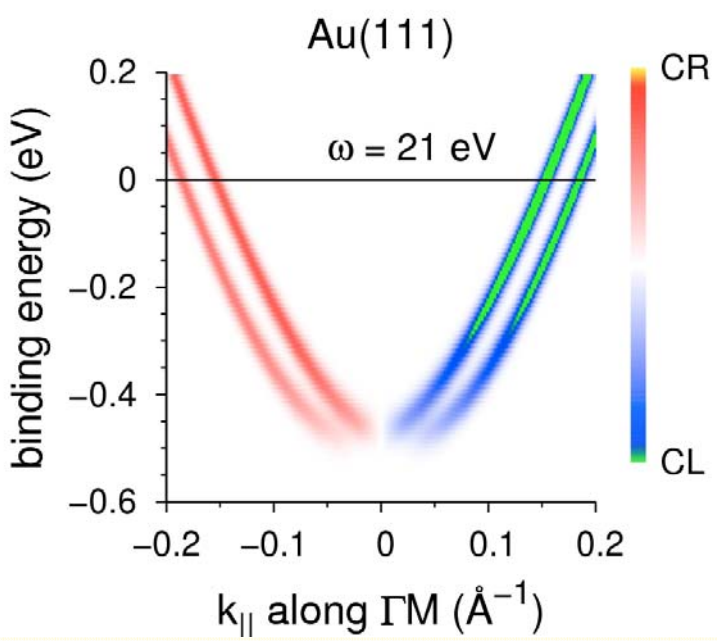


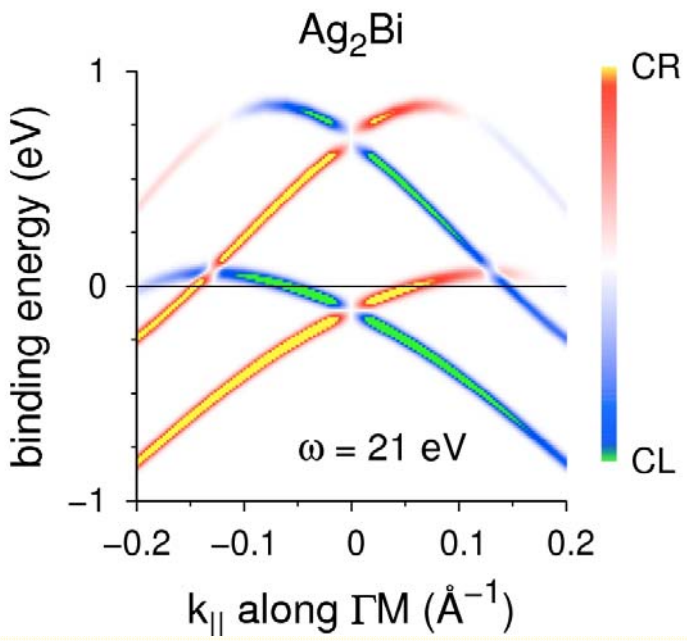
SURFACE STATES: CONCLUSIONS

- Rashba model is not applicable to realistic crystals: the splitting cannot be understood in terms of non-relativistic wave functions.

- However, it demonstrates the role of crystal potential apart from the gradient term: it affects the splitting by modifying the wave functions.

SURFACE STATES: PHOTOELECTRON SPECTROSCOPY



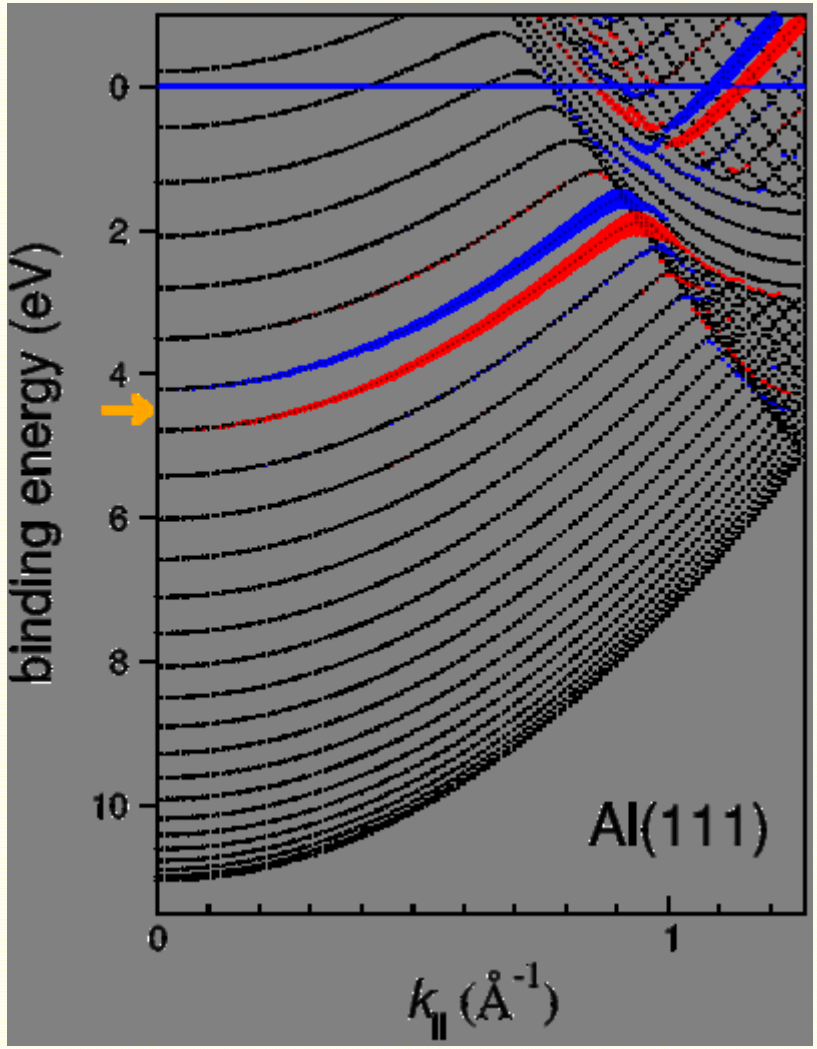


Circular dichroism in photoemission from spin-orbit split surface states: *ab initio* calculation.

Quantum well states: spin-polarization at the surface

spin ↓ spin ↑

Aluminum slab: finite-size quantization of the nearly-free-electron states is accompanied by the spatially local spin polarization.



Spectral distribution of spin polarization

EK and E.V. Chulkov, Phys. Rev. B **83**, 155401 (2011)

bulk continuum states: spin-polarization at the surface

Surface Polarization in the Rashba Model

For a system with one-dimensional crystallinity, $V(\mathbf{r}_\parallel, z) = V(z)$, the two-component Hamiltonian reads

$$\hat{H} = -\Delta + V + \frac{\alpha^2}{2} V_z' \begin{pmatrix} 0 & -i\hat{p}_x - \hat{p}_y \\ i\hat{p}_x - \hat{p}_y & 0 \end{pmatrix}.$$

In the Schrödinger equation for a Bloch function $\psi(\mathbf{r}) = \psi(z) e^{i\mathbf{k}_\parallel \mathbf{r}_\parallel}$ the two spin components ψ^+ and ψ^- along the axis perpendicular to both $\mathbf{z}$ and $\mathbf{k}_\parallel$ separate:

$$-\psi^{+\prime\prime} + (V+\zeta)\psi^+ = E\psi^+$$
$$-\psi^{-\prime\prime} + (V-\zeta)\psi^- = E\psi^-.$$

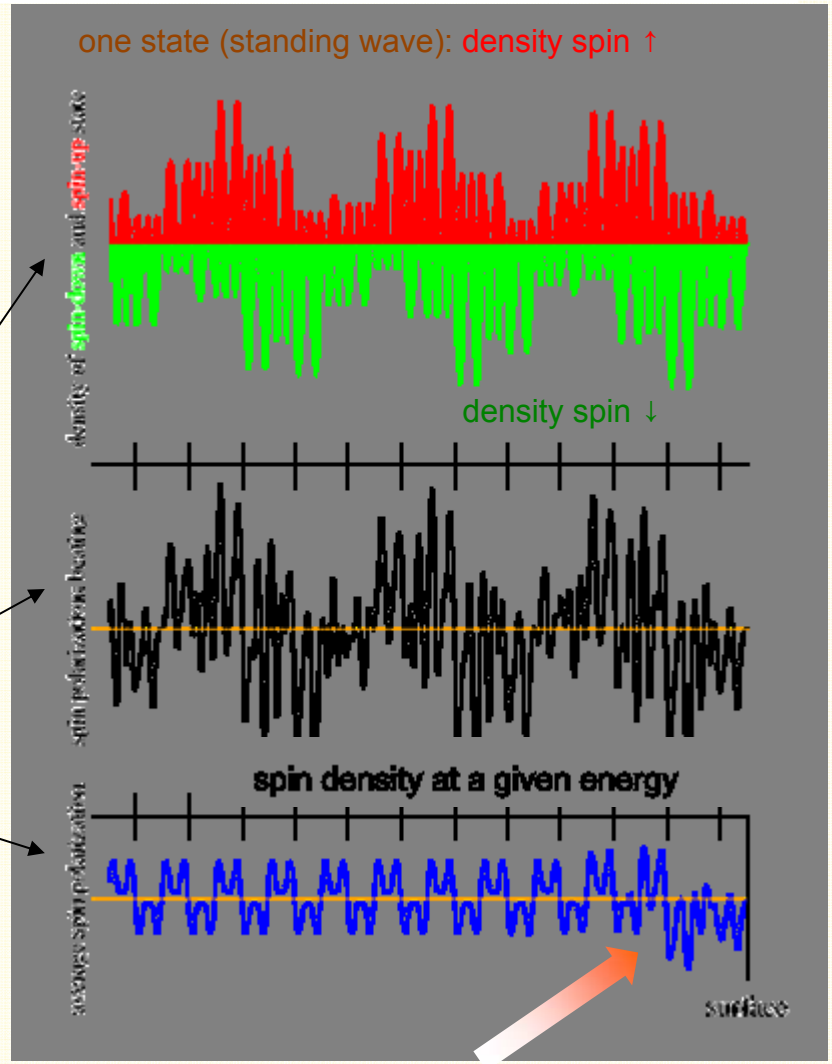
The two scalar wave functions ψ^+ and ψ^- feel different effective potentials, so the reflection of the incident wave from the surface depends on its spin.

Because of the beating effect between the incident and the reflected wave the spin density due to the two waves does not have the lattice periodicity.

However, after the integration over dk_z the beating decays into the bulk as $1/z$. Thus, the $\mathbf{k}_\parallel$-resolved polarization is finite only at the surface.

Owing to the surface sensitivity of the photoemission, the Rashba-type spin polarization of the bulk continuum states can be observed in angle-resolved measurements.

Spin density distribution in a semi-infinite crystal



spin density integrated over a k_z interval

EK and E.V. Chulkov, Phys. Rev. B **83**, 155401 (2011)

one-step theory: first order perturbation theory → Fermi golden rule

First-order perturbation theory:

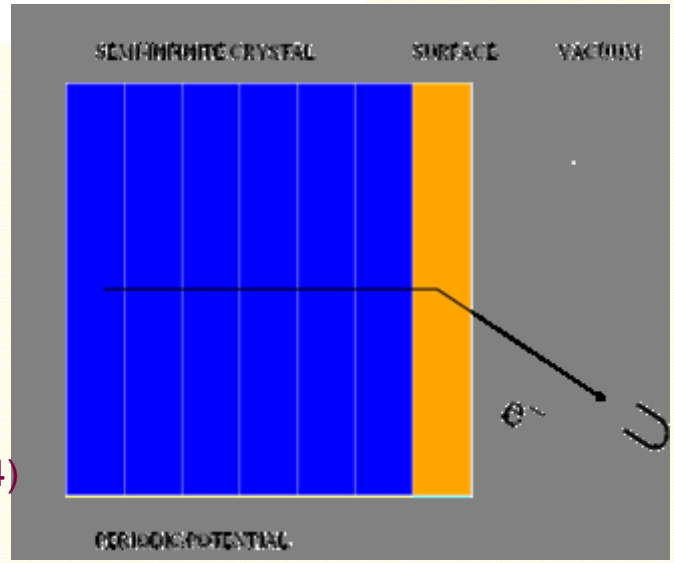
$$\psi(\vec{r};\epsilon+\hbar\omega) = \int d\vec{r}\,'\, G(\vec{r},\vec{r}\,';\epsilon+\hbar\omega)\,[-i\nabla]\,\phi(\vec{r}\,';\epsilon)$$

Asymptotics at the detector $r \to \infty$

$$\begin{aligned}\psi(\vec{r};\epsilon+\hbar\omega) &= \int d\vec{r}\,'\, \Phi_{\mathrm{LEED}}(E_{\mathrm{fin}},\vec{r}\,')\,[-i\nabla]\,\phi(\vec{r}\,') \\ &= \langle\, \mathrm{LEED}^* \,|\, -i\nabla \,|\, \phi \,\rangle\end{aligned}$$

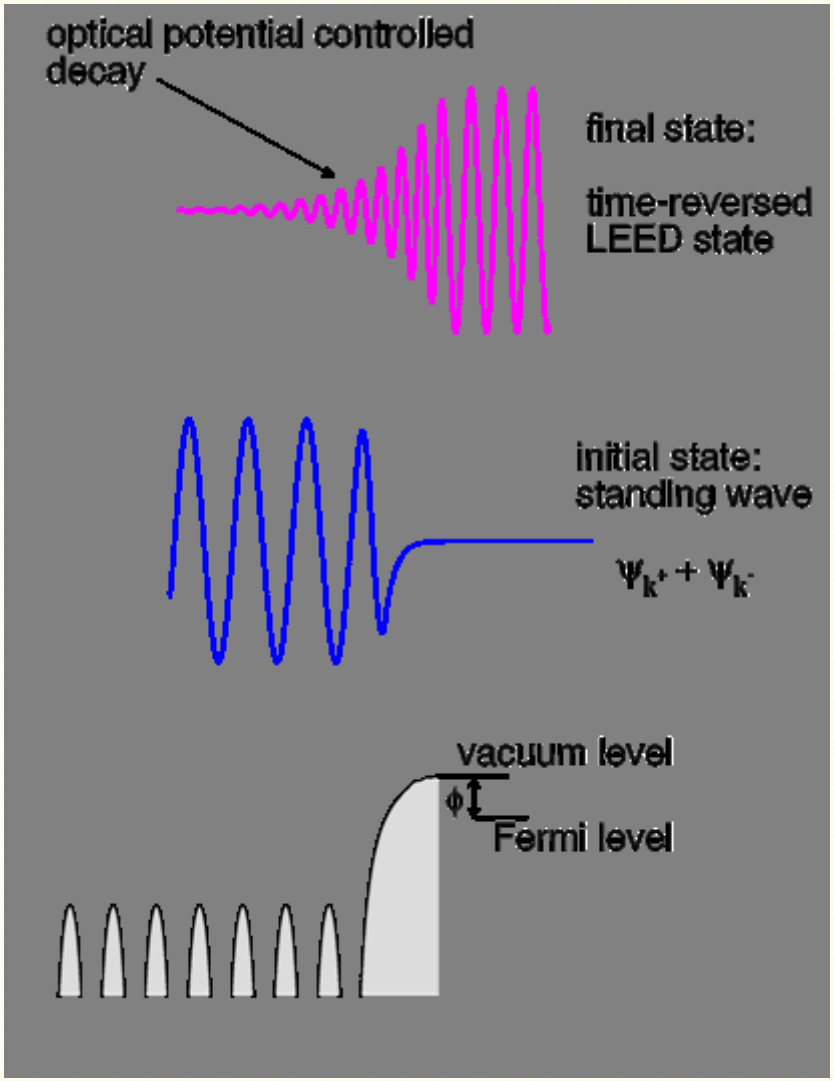
Time reversed LEED state

= final state (loosely speaking)

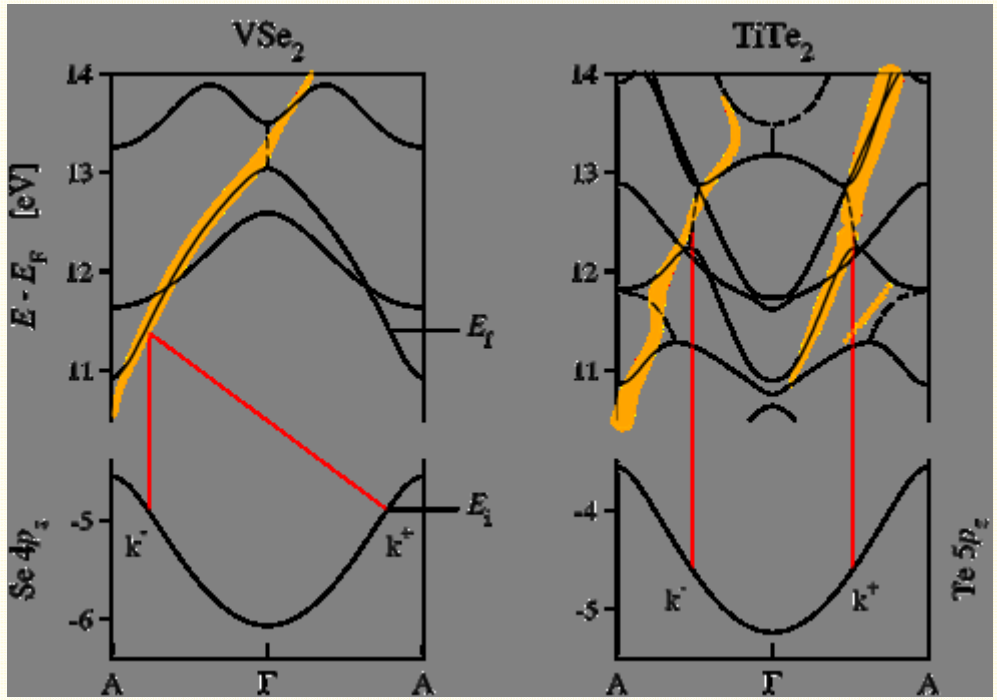


G.D. Mahan, Phys. Rev. B **2**, 4334 (1970)
P.J. Feibelman and D.E. Eastman, Phys. Rev. B **10**, 4932 (1974)

One-step theory has been implemented within the multiple-scattering method [J.B. Pendry, Surf. Sci. **57**, 679 (1976)] and within the band structure formalism [EK, Phys. Rev. B **70**, 2453225 (2004)]



Conducting complex band structure

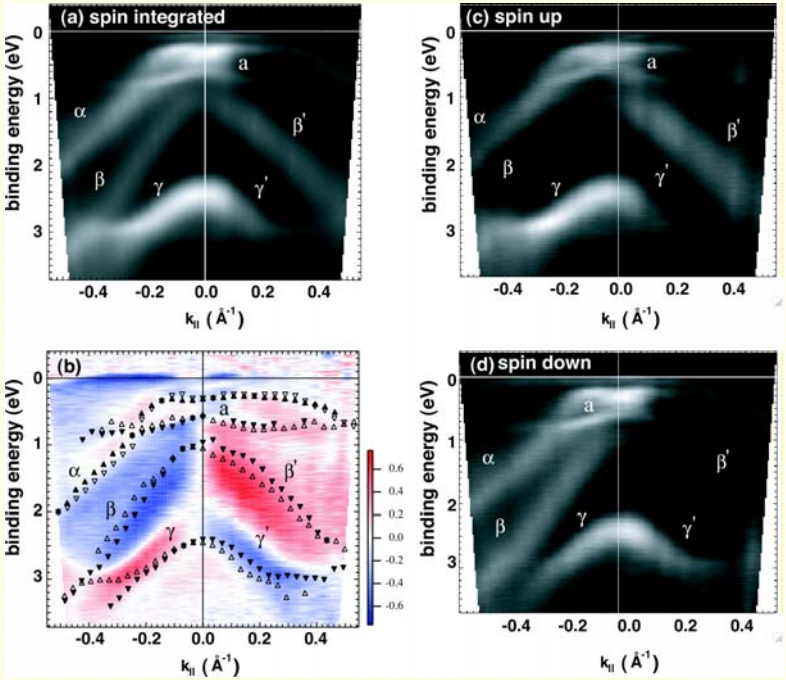


$k_\parallel$ projected band structure

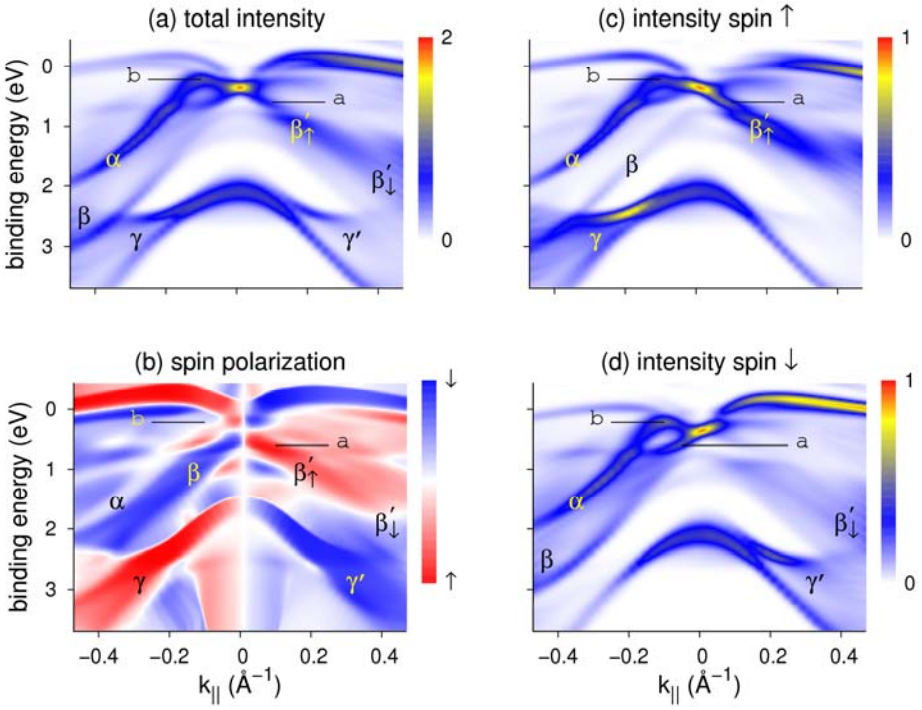
Spin-resolved photoemission from Bi(111): polarization without energy splitting

spin-resolved energy-momentum photoemission distribution : line *MΓM*

experiment

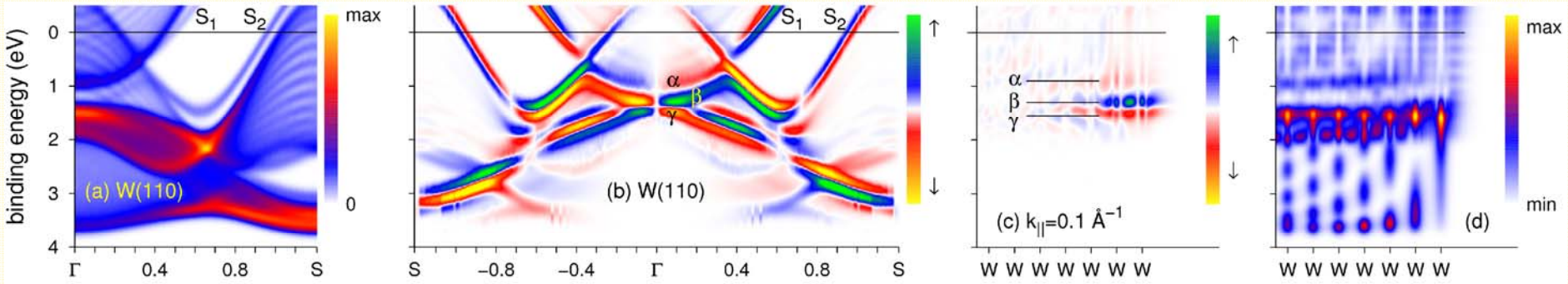


theory



A. Kimura, E.E. Krasovskii, R. Nishimura, K. Miyamoto, T. Kadono, K. Kanomaru, E.V. Chulkov, G. Bihlmayer, K. Shimada, H. Namatame, and M. Taniguchi, Phys. Rev. Lett. **105**, 076804 (2010)

Spin polarization of the density of states in bulk continuum: W(110)



W(110) surface:

(a) Energy-momentum DOS distribution for $\mathbf{k}_\parallel$ along the $\bar{\Gamma}\bar{S}$ line of SBZ.

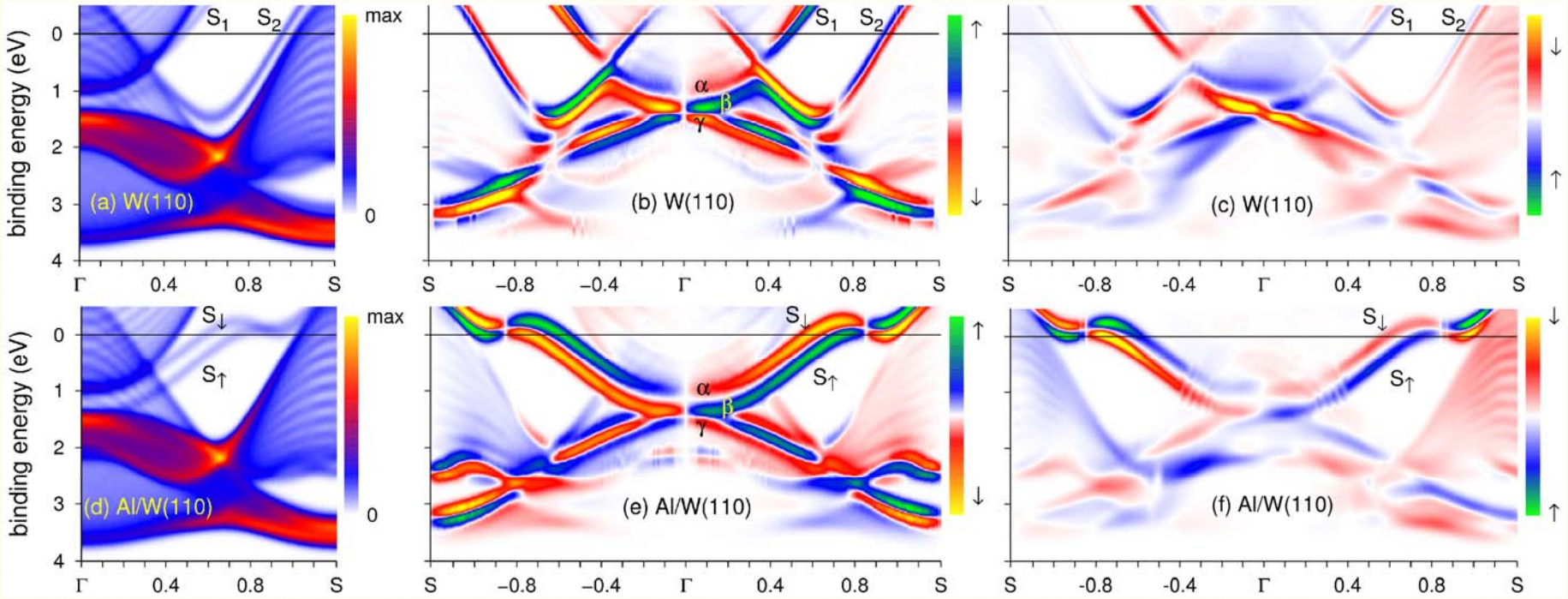
(b) Energy-momentum distribution of spin polarization along $\bar{\Gamma}\bar{S}$.

(c) Local depth-resolved $k_\parallel$ projected net spin density $\rho^{\uparrow}_{\mathbf{k}_\parallel} - \rho^{\downarrow}_{\mathbf{k}_\parallel}$ for $k_\parallel = 0.1$ Å^{-1}.

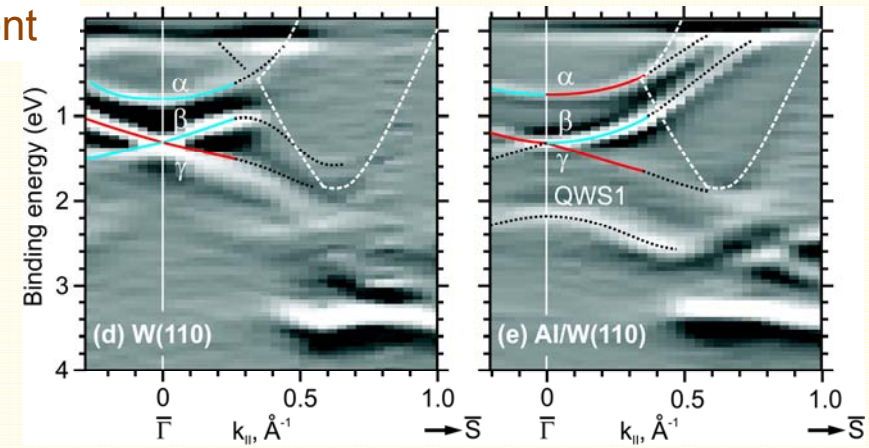
(d) Local depth-resolved $k_\parallel$ projected DOS for $k_\parallel = 0.1$ Å^{-1}.

$$\rho^{\sigma}_{\mathbf{k}_\parallel}(z, E) = \int d\mathbf{r}_\parallel \sum_{\lambda} |\psi^{\sigma}_{\lambda\mathbf{k}_\parallel}(\mathbf{r})|^2 \delta(E_{\lambda\mathbf{k}_\parallel} - E).$$

Surface polarization and spin-resolved photocurrent: W(110) and Al/W(110)



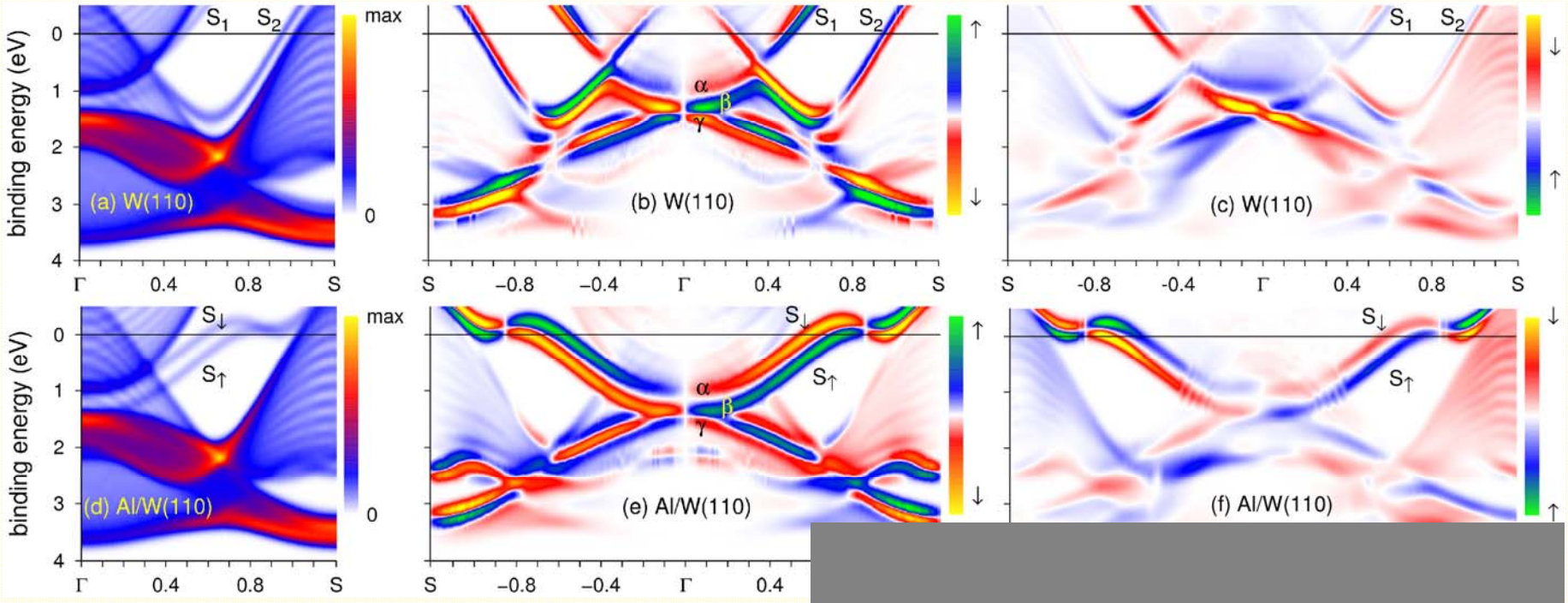
experiment



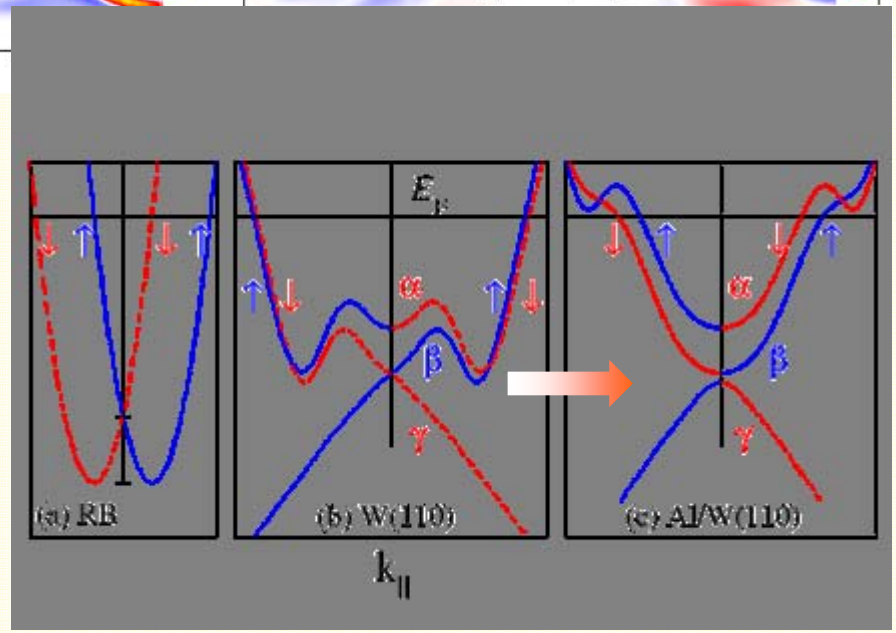
Polarization of the photocurrent does not follow the polarization of the surface DOS.

A.G. Rybkin, EK, D. Marchenko, E.V. Chulkov,
E.V. Varykhalov, O. Rader, and A.M. Shikin, PRB **86**, 035117 (2012)

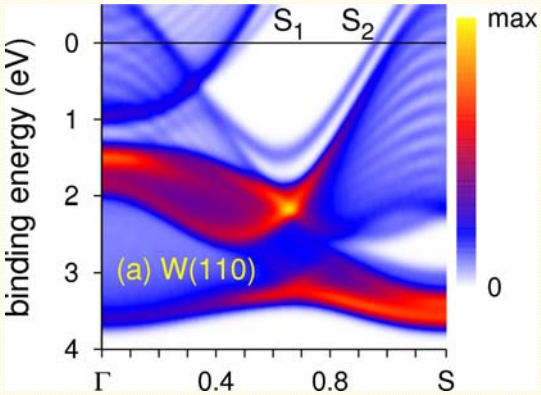
Surface polarization and spin-resolved photocurrent: W(110) and Al/W(110)

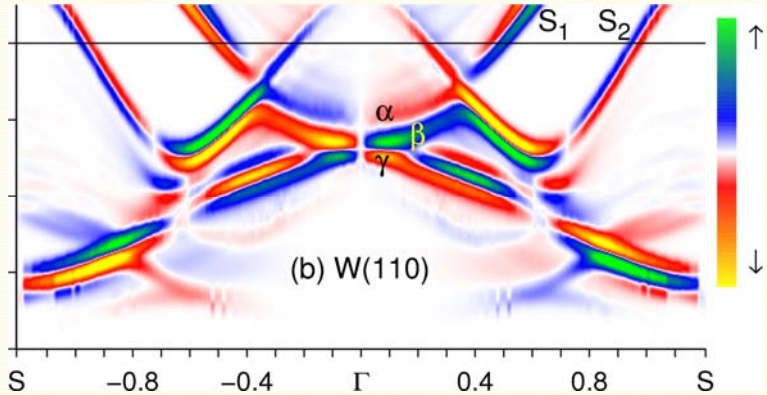


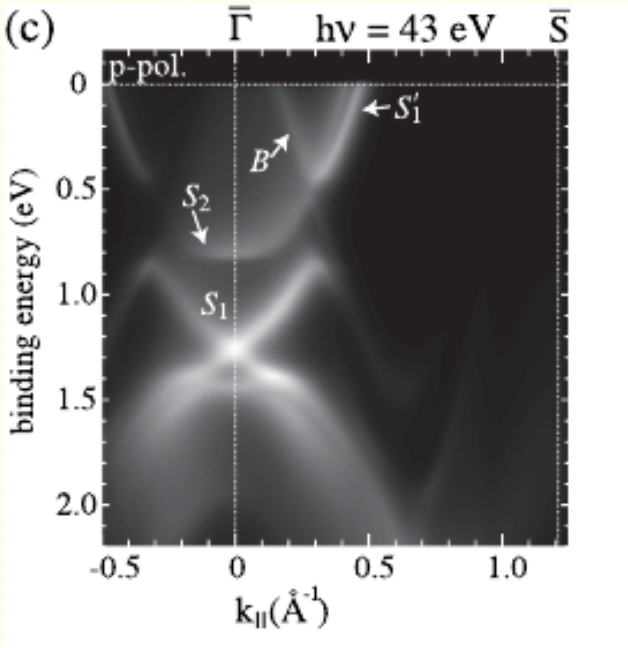
dispersion of the polarization branches changes upon the deposition of an Al monolayer



Spin-polarization of the density of states in bulk continuum: W(110)







K. Miyamoto, A. Kimura, K. Kuroda, T. Okuda, K. Shimada, H. Namatame, M. Taniguchi, and M. Donath, Phys. Rev. Lett. 108, 066808 (2012)

CONCLUSIONS

The Rashba effect leads to the spin-orbit splitting of the surface states as well as to the polarization of the bulk states.

The reality is fundamentally different from the Rashba model in view of the decisive role of the in-plane scattering whereby the splitting is determined by non-relativistic velocity.

Thank you
for your attention!