

Evolution of topological surface states of thin HgTe-films with film thickness

March 25, 2017

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2017-03-25

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Hello, my name is Tamara Szecsey and I will now give you a talk about my bachelor thesis topic, the evolution of topological surface states of thin HgTe-films with film thickness.

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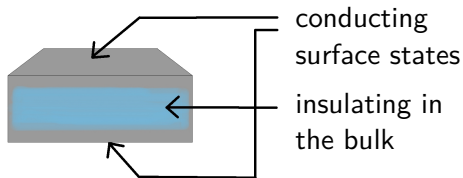
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Introduction

HgTe is a II-VI semiconductor and a topological insulator (TI).¹



TIs are interesting because:

- ▶ spin-momentum locking
- ▶ protected surface states

Calculations were performed using density functional theory (DFT) through FHI-aims.

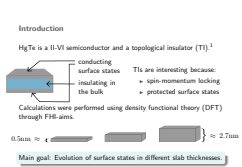


Main goal: Evolution of surface states in different slab thicknesses.

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Introduction

Introduction



HgTe belongs to the class of mercury-based II-VI(6) semiconductors which appear in zinc-blende structure. It is additionally found to be a topological insulator.

A topological insulator is a material which is insulating in its interior, also called the bulk of a material, and that develops conducting states at the surface.

They are very attractive for potential applications because the spin and the momentum of the electrons at the conducting surfaces are locked. This means, the spin is always perpendicular to the direction of motion of those electrons. The spin-momentum locking makes sure that the surfaces are protected if time-reversal symmetry is preserved. In other words the surface states remain, even for non-magnetic impurities. The calculations I performed were ab-initio calculations and therefore I used the density functional theory with the exchange-correlation function method PBE through FHI-aims.

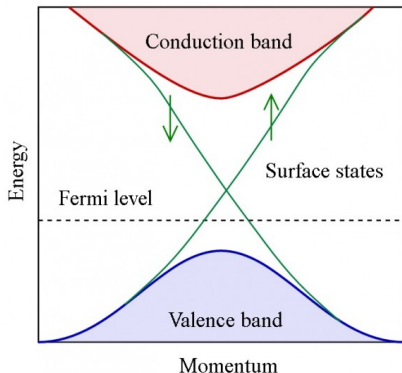
HgTe was examined in thin films from approximately 0.5 nm to 2.7 nm, which are 4 to 17 layers of atoms. Surfaces can only be examined in one direction at once. Because otherwise it would went beyond the scope of a bachelor thesis, we chose just one direction of observance, namely the (001) direction.

The main goal this thesis pursued was examining the evolution of topological surface states for different slab thicknesses. Therefore I will now explain the theory behind the realization of this examination.

Theory: Topological insulator

2005 Kane and Mele found another class of material:
the topological insulator (TI).

spin-orbit coupling → band inversion → Dirac cone



2D TI:

have quantum spin edge states
found in graphene and HgTe
quantum wells.

3D TI:

strong and weak ones
HgTe is semi metal but under
strain Γ_6 and Γ_8 bands can close
up at Fermi level.

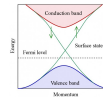
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Theory

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3D TI: strong and weak ones. HgTe is semi metal but under strain Γ_6 and Γ_8 bands can close up at Fermi level.

Besides from insulators and conductors, Kane and Mele 2005 found another class of material which is the so-called topological insulator. Most of the unusual properties come from the including of the spin-orbit coupling. This produces the spin-momentum locking mentioned earlier and can lead to band inversion. The spin-momentum locking and time-reversal symmetry prevent backscattering, because for two opposite momentums, the spin is also opposite and the states interfere destructively. In other words, the surface states are protected by time-reversal symmetry. If the surface states close up because of band inversion then a so-called Dirac cone arises like seen in this picture from wikipedia. Here we see the momentum plotted against the energy near Fermi level. The blue line is the valence band and the red one is the conduction band. The surface states in green have a spin locked to their momentum and are forming a Dirac cone because their bands are inverted.

In 2D there were found topological surface states in graphene and HgTe quantum wells which are called Quantum spin edge states based on the Quantum spin hall effect. These quantum wells have non-trivial topological surface states under a certain critical thickness but become trivial insulators as soon as they pass this critical thickness. 3D topological insulators are distinguishable into strong and weak topological insulators where the number of dirac cones is odd for strong and even for weak ones. HgTe normally is a semi metal but under strain its Γ_6 and Γ_8 bands can close up at Fermi level, which means its surface states become topological.

Theory: Crystal and surface description part 1

Translation Vector: $\mathbf{R}_i = x_i \mathbf{a}_1 + y_i \mathbf{a}_2 + z_i \mathbf{a}_3$

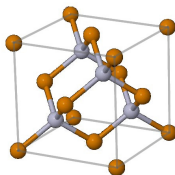
contains basis for lattice forming a unit cell.

Smallest primitive unit cell is the Wigner Seitz cell.

Bravais lattice

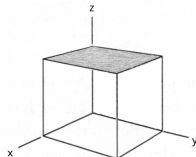
fcc lattice with two atomic basis \rightarrow diamond or zinc-blende structure

Miller indices: (hkl)



	x	y	z
\mathbf{a}_1	0	$\frac{a}{2}$	$\frac{a}{2}$
\mathbf{a}_2	$\frac{a}{2}$	0	$\frac{a}{2}$
\mathbf{a}_3	$\frac{a}{2}$	$\frac{a}{2}$	0
Te	0	0	0
Hg	$\frac{a}{4}$	$\frac{a}{4}$	$\frac{a}{4}$

$$h : k : l = \frac{1}{x} : \frac{1}{y} : \frac{1}{z}$$



(001)

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└ Theory

└ Theory: Crystal and surface description part 1

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Translation Vector: $\vec{R}_i = x_i \vec{a}_1 + y_i \vec{a}_2 + z_i \vec{a}_3$

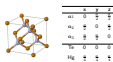
contains basis for lattice forming a unit cell.

Smallest primitive unit cell is the Wigner Seitz cell.

Bravais lattice

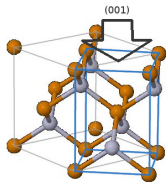
fcc lattice with two atomic basis \rightarrow diamond or zinc-blende structure

Miller indices: (hkl)



Theory: Crystal and surface description part 2

Basis for (001) direction of zinc-blende structure:



	x	y	z
a_1	$\frac{a}{\sqrt{2}}$	0	0
a_2	0	$\frac{a}{\sqrt{2}}$	0
a_3	0	0	a

	x	y	z
Te	0	0	0
Hg	$\frac{a}{2\sqrt{2}}$	0	$\frac{a}{4}$
Te	$\frac{a}{2\sqrt{2}}$	$\frac{a}{2\sqrt{2}}$	$\frac{a}{2}$
Hg	0	$\frac{a}{2\sqrt{2}}$	$\frac{3a}{4}$

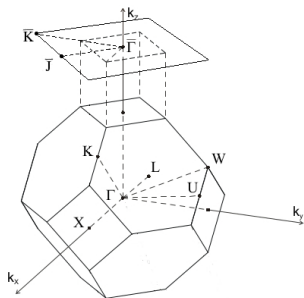
Reciprocal lattice: $e^{i\mathbf{K}\mathbf{R}} = 1$

\mathbf{K} is reciprocal translation vector.

First Brillouin zone (BZ) is Wigner Seitz cell for reciprocal space.

Super symmetrical points:

$$\bar{\Gamma} = 0; \quad \bar{J} = \frac{1}{2}\mathbf{b}_1; \quad \bar{K} = \frac{1}{2}\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_2$$



Theory: Surface modeling

Termination

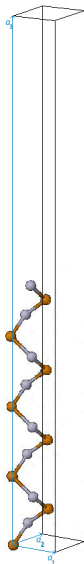
Two surfaces with symmetric Hg-Hg, Te-Te terminations or antisymmetric Te-Hg terminations.
Add hydrogen atoms in order to saturate dangling bonds.

Number of layers

Atoms with same z component are in the same layer.
Odd for symmetric, even for antisymmetric termination.
I studied 3 different thicknesses for each termination.

Supercell approach

Infinite repetition only possible in all directions.
In order to avoid interactions between slabs in k_z direction: add vacuum space.



Theory: Density functional theory (DFT)

First Hohenberg-Kohn Theorem:

$\rho(\mathbf{r})$ can be uniquely converted into the $V_{\text{ext}}(\mathbf{r})$

Second Hohenberg-Kohn Theorem:

Ground state energy can be expressed in a density functional:

$$E^{\text{HK}}[\rho(\mathbf{r}); v_{\text{ext}}(\mathbf{r})] = T_0[\rho] + V_{\text{H}}[\rho] + \int v_{\text{ext}}(\mathbf{r})\rho(\mathbf{r})d\mathbf{r} + E_{\text{xc}}[\rho]$$

Kohn-Sham equation

Minimizing $E^{\text{HK}} \rightarrow$ Kohn-Sham eigenfunctions $\phi_i(\mathbf{r})$:

$$E_0[\rho_0] = E_{\text{nucl}} + E_{\text{kin}} + E_{\text{H}} + E_{\text{xc}}$$

Perdew-Burke-Ernzerhof (PBE) functional

$$E_{\text{xc}}^{\text{PBE}} = \int d^3r \rho(\mathbf{r}) \epsilon_{\text{xc}}^{\text{PBE}}(r_s(\mathbf{r}), s(\mathbf{r}), \zeta(\mathbf{r}))$$

Theory: Spin-orbit coupling

Dirac equation:
$$(c\boldsymbol{\alpha} \cdot \mathbf{p} + c^2(\beta - 1) + V) \Psi = \epsilon \Psi$$

Separate Ψ into two spinors:
$$\Psi = \begin{pmatrix} \Psi_L \\ \Psi_S \end{pmatrix}$$

Substitute and dissolve:

$$\left(\mathbf{p} \frac{c^2}{2c^2 + \epsilon - V} \mathbf{p} + i\mathbf{p} \frac{c^2}{2c^2 + \epsilon - V} \times \mathbf{p} \cdot \boldsymbol{\sigma} + V \right) \Psi_L = \epsilon \Psi_L$$

First part with V is relativistic Schrödinger equation.

Expanding in $\frac{\epsilon - V}{2c^2}$ in zeroth order gives non-relativistic Schrödinger equation.

Expanding just second part in first order gives:

$$V_{SOC} = \frac{i}{4c^2} \mathbf{p} V \times \mathbf{p} \cdot \boldsymbol{\sigma}$$

bla2

Conclusion

blub2