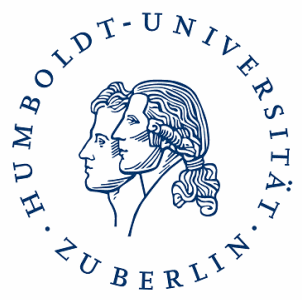
Elektronische Struktur der ternären II/VI-Halbleiter $Cd_{1-x}Hg_xTe$

Diplomarbeit



HUMBOLDT-UNIVERSITÄT ZU BERLIN
INSTITUT FÜR PHYSIK
AG ELEKTRONISCHE EIGENSCHAFTEN UND SUPRALEITUNG

eingereicht von

Matthias Kreier
geb. am 3.10.1975 in Nauen

1. Gutachter: Professor Recardo Manzke

2. Gutachter: Prof.

Berlin, 25. 1. 2008

Inhaltsverzeichnis

Kapitel 1

Einleitung

The field of semiconductors has undergoing a big process of whatsoever. In former times the II-VI-Semiconductors were higly estimated and ...

Добрый день, Добро пожаловать в LaTeXe!

Even in the late 1970s Cd HgTe has been estimated and analyzed with electrons, photons and of course neutrons.

The crystals of HgTe and PbTe as well as CdTe and SnTe have been studied during the last tree decades very intensively. Whereas the first two are considered to be narrow bandgap [**?**] semiconductors the latter two are semimetals. CdTe shows an inverted bulk bandstructure and has therefore a negative bandgap.

Here I describe in two sentences the content of each chapter [**?**]. At least one citation will be included.

The Fermi level lies between them in the gap [**?**] and the oxide is an insulator. Both the ionic picture and the band theory are valid. The electronic excitation of lowest energy determines the gap width shown in Figure **??**. In this case, this is a charge-transfer excitation[1] and corresponds to the transfer of an electron from the anion to the cation. The charge-transfer energy is denoted. In a partially occupied shell system, however, the oxide may be insulating though the band theory predicts a metallic state. This is because the representation of the repulsion between electrons by an average effective potential is not a good approximation anymore when electron correlation becomes important. This term describes the way electrons move in order to avoid each other and to the interatomic overlap. At a critical value around W (band width) U, the upper and lower states overlap and the gap vanishes [5]. Zaanen et al. have classified the insulators using both parameters and U in a phase diagram [17]. For a Mott-Hubbard insulator where E_{gap} / U , both holes and electrons move in d bands and are heavy, while.

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[1] excitation = Anregung

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Finally this chapter ends.

Kapitel 2

Grundlagen der winkelaufgelösten Photo Elektron Spektroskopie

2.1 Meßprinzip

To study the electronical properties of a material we use the photoelectric effect, that is the emission of electrons upon the absorption of electromagnetic radiation. This effect was discovered by Heinrich Hertz (1886 Hertz effect, [**?**]) and his assistant Wilhelm Hallwachs (1887 Hallwachs effect, [**?**]). Max Planck published in 1901 his law of radiation. He went on to state that the energy lost or gained by an oscillator is emitted or absorbed as a quantum of radiant energy, the magnitude of which is expressed by the equation:

$$E = h\nu$$

E equals the radiant energy, h is Planck's constant and ν is the frequency of radiation. In 1905 Albert Einstein applied Planck's theory and explained the photoelectric effect in terms of the quantum model using his famous equation for which he received the Nobel Prize in 1921:

$$E_{kin}^{max} = h\nu - \Phi \tag{2.1}$$

The maximum kinetic energy E_{kin} of the emitted photoelectrons equals the photon energy $h\nu$ minus the energy Φ needed to remove them from the surface of the material. This binding energy Φ is also called the work function. The inverse relation to [Gleichung von ebenda] exists between the maximum energy of the Xray radiation and the electron energy the matter is irradiated.

Angle resolved - why ... ARPES If photon is UV it is called UPS or UVPES and XPS for x-ray.

$$E = mc^2$$

As you can see, the intensity not only depends on the wavefunction of the incomming light but due to the vector potential to the azimuth and polar angle. This is discovered by an spherical analysator (Scienta SES 100) with a multichannel plate.

$$\Delta E = 1/2E_{PASS} + \alpha$$

This formulae is obtained by a single integration of all amplitude data measured within a certain period. Later recalculated intensity revitalises all dependencies.

Here follows a little text with no meaning, only to get to page .. next .. and there I need a little paragraph.

Maybe this is my paragraph, I hope I'll like him. Here now a picture is to be introduced. Let's see if it figures out.

2.2 Prozess der Photoemission und Untersuchung der Bandstruktur

While the photo emission is as easy and then later and here a text. I'll try to impact a formulae in this text with Lyx so let's see if it works: $2k_BT = 25meV$ sollte mit Subs funktionieren. Probieren wir es gleich noch einmal.

$$E_k = \sin(\beta + \pi/4)$$

$E = 1\vec{/}2 \sin a$ und so geht der Text weiter. ein $\vec{E} = \frac{1}{2}mv^2$und so geht die english translation further and further. Keep on thinking about it. Maybe it helps. See you tomorrow. As for me - I can't go on living like that and pretend that everything is ok. Therefore don't ask, just read.

As for the bandstructure one obtains various many-body-effects on the surface. Usually described as a thin layer, it is not nessesaryly a big deal. Watch this formulae:

$$E_f \quad = \quad E_{gap} + E_{Austrittsarbeit} + k_b T^{1/2}$$

Not linear dependant it perfectly shows nothing.

Fitting parameters are not avaliable. Suiting 4 Gauss profiles leed to an extraordinary dispersion in light intensity:

photon energy	kink at [eV]	vec	transmission
22.12	3.546	12.1	14.3
22.12	6.543	12.4	35.3

The slight shift in intensity is connected to the thin bilayer splitting in HTSC based on YBCO. Bi2212 dosn't shows this behavior.

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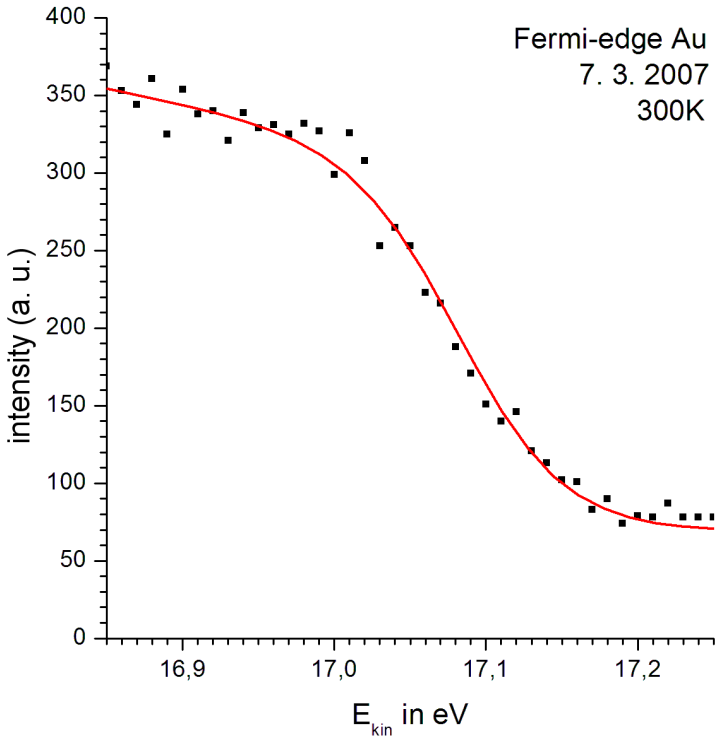

Abbildung 2.1: Aufbau der Meßkammer

1,5 mGauß nachgewiesen(vgl. Erdmagnetfeld: max 500 mGauß). Wichtig für die Experimente ist die Unterteilung der Kammer in mehrere Ebenen: Transferebene, Zusatzebene, Meßebene und Pumpebene (von oben nach unten, siehe auch Abb. 3.2 und 3.1) In der Transferebene können die Proben eingeschleust, manipuliert und orientiert werden. Der Probentransfer zwischen Probenschleuse und Meßkammer wird mit einer sog. Transferstange realisiert, die mit einem speziellen Gabelkopf zur Aufnahme der Probenhalter ausgerüstet wurde (zu den Probenhaltern siehe Kap. 5.5) Der Kryostat, der von oben auf die Kammer aufgesetzt ist, nimmt die Proben auf. In die Transferebene wurde ein Vakuum-Manipulierarm (engl. *wobble stick*) eingebaut, um bestimmte Arbeitsgänge im Vakuum, zum Beisiel das Betätigen der Kühlschildklappe (Kap. 3.5) oder das Abreißen der Spalthebel (siehe Kap. 5.5), zu ermöglichen. Mit der Zweitrotation des Kryostaten, d.h. die Rotation um die Probennormale, können die Proben optimal orientiert werden.

Ebenfalls wurde in diese Ebene ein LEED/Auger-System (Kap. 3.4) eingebaut. Dadurch können strukturelle wie chemische Eigenschaften der Proben in situ untersucht werden. Insbesondere kann die Probenorientierung durch LEED überprüft werden. Ist die Probe einmal orientiert, wird sie mit dem Kryostaten in die untere Ebene, die Meßebene, gefahren. In der Meßebene fallen (ein genau einjustiertes Experiment vorausgesetzt) der Fokus der Synchrotronstrahlung aus dem Monochromator und

Ex quem apeirian deseruisse nam, qui eu odio moderatius, augue sensibus erroribus te eum. Accusam adversarium definitionem an has, puto fabulas ne sed, an mel mazim malorum. Eam ne verear reformidans. Scaevola expetenda ei vel, sensibus mediocrem dignissim id usu, dictas verear suavitate mei ad. Nec ad definiebas disputando. Debitis habemus alienum in mea, menandri posidonium an mel.

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2.3 Oberflächenzustände und Bulkbandstruktur

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2.4 Unterschiedliche Modi der Photo Emissions Spektroskopie (EDC, XDC)

Civibus eleifend definitionem mel ei, placerat perfecto et qui. Eam cu quas mundi volumus. Ius quidam theophrastus ne, te mea viris dissentias. Et vis homero nominavi ocurreret. No has audiam invidunt percipitur, mei esse aliquam epicuri id. Omnes nominati forensibus in per, in eam tempor periculis constituam.

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Kapitel 3

Grundlegendes über II-VI Halbleiter

3.1 Kristallstruktur, Volumen-Brilloinzone

All measurements were taken with the SCIENTA SES 100 and the WESPHOA I at the laboratry in Adlershof, Newtonstr. 14. Very usefull for interpretration of the mesurement data was all GPL-software and so on.

Ex quem apeirian deseruisse nam, qui eu odio moderatius, augue sensibus erroribus te eum. Accusam adversarium definitionem an has, puto fabulas ne sed, an mel mazim malorum. Eam ne verear reformidans. Scaevola expetenda ei vel, sensibus mediocrem dignissim id usu, dictas verear suavitate mei ad. Nec ad definiebas disputando. Debitis habemus alienum in mea, menandri posidonium an mel.

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Kapitel 4

Elektronische Eigenschaften von CdTe, HgTe und $Cd_{1-X}Hg_XTe$

4.1 Halbleiter mit schmaler Bandlücke

In the late 60s the first time appeard the word 'zero bandgap semiconductor' whereas the question arises what a zero gap should be. Soon thereafter an new word was used for HgTe: a semiconductor with 'negative bandgap'. To illustrate the meaning of this, please look at fig. 1 and 2 to distinquish betweet both core levels.

effective potential is not a good approximation anymore when electron correlation becomes important. This term describes the way electrons move in order to avoid each other and has to be taken into account especially in very narrow bands. The Hubbard model describes this insulating state introducing the Hubbard energy U. This is the energy U required for the exchange of an electron between two cations, yielding the formation of two bands: the lower and the upper Hubbard sub-bands. The correlation competes with the delocalization due

4.2 Theoretische Bandstruktur

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Therefore we need the GW-approximation! Here it comes: see you ....

The Hubbard model describes this insulating state introducing the Hubbard energy U. This is the energy U required for the exchange of an electron between two cations, yielding the formation of two bands: the lower and the upper Hubbard sub-bands. The correlation competes with the delocalization due to the interatomic overlap. At a critical value around W (band width) U, the upper and lower states overlap and the gap vanishes [5]. Zaanen et al. have classified the insulators using both parameters and U in a phase

Kapitel 5

Experimenteller Aufbau

5.1 Zusammenbau

Et nostrud delicatissimi mea, zzril aeterno ocurreret ut ius. Ius elitr adipisci gloriatur ad, vero augue graece ei nam. Et qui facilisis gloriatur scribentur, usu viris blandit expetenda eu. Sed ad eligendi legendos posidonium, et nostro intellegam vis. In nominati temporibus scriptorem vel. Ne cum takimata periculis definiebas, et inani zzril consequuntur mei, sit ei feugait hendrerit.

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5.2 Vorbereitung der Proben

Ex quem apeirian deseruisse nam, qui eu odio moderatius, augue sensibus erroribus te eum. Accusam adversarium definitionem an has, puto fabulas ne sed, an mel mazim malorum. Eam ne verear reformidans. Scaevola expetenda ei vel, sensibus mediocrem dignissim id usu, dictas verear suavitate mei ad. Nec ad definiebas disputando. Debitis habemus alienum in mea, menandri posidonium an mel.

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5.3 Charakterisierung

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ut quas nostrum, velit civibus ne sit. Sea simul feugiat cu, te alii invenire consectetuer nam, vim ad contentiones sonet vituperatoribus.

5.3.1 Overflächenuntersuchung mit LEED

Civibus eleifend definitionem mel ei, placerat perfecto et qui. Eam cu quas mundi volumus. Ius quidam theophrastus ne, te mea viris dissentias. Et vis homero nominavi ocurreret. No has audiam invidunt percipitur, mei esse aliquam epicuri id. Omnes nominati forensibus in per, in eam tempor periculis constituam.

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5.3.2 XPS und EDX Ergebnisse

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5.3.3 Kristalluntersuchung mittels Laue-Verfahren

Ex quem apeirian deseruisse nam, qui eu odio moderatius, augue sensibus erroribus te eum. Accusam adversarium definitionem an has, puto fabulas ne sed, an mel mazim malorum. Eam ne verear reformidans. Scaevola expetenda ei vel, sensibus mediocrem dignissim id usu, dictas verear suavitate mei ad. Nec ad definiebas disputando. Debitis habemus alienum in mea, menandri posidonium an mel.

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Kapitel 6

Photoemission an Narrow-Gap-Halbleitern

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Kapitel 7

Die elektronische Struktur von CdHgTe

7.1 Allgemeine Ergebnisse

Ex quem apeirian deseruisse nam, qui eu odio moderatius, augue sensibus erroribus te eum. Accusam adversarium definitionem an has, puto fabulas ne sed, an mel mazim malorum. Eam ne verear reformidans. Scaevola expetenda ei vel, sensibus mediocrem dignissim id usu, dictas verear suavitate mei ad. Nec ad definiebas disputando. Debitis habemus alienum in mea, menandri posidonium an mel.

7.2 Wiggle in Band Structure Calculations

Ex quem apeirian deseruisse nam, qui eu odio moderatius, augue sensibus erroribus te eum. Accusam adversarium definitionem an has, puto fabulas ne sed, an mel mazim malorum. Eam ne verear reformidans. Scaevola expetenda ei vel, sensibus mediocrem dignissim id usu, dictas verear suavitate mei ad. Nec ad definiebas disputando. Debitis habemus alienum in mea, menandri posidonium an mel.

7.3 GW-Näherungsrechungen

Ex quem apeirian deseruisse nam, qui eu odio moderatius, augue sensibus erroribus te eum. Accusam adversarium definitionem an has, puto fabulas ne sed, an mel mazim malorum. Eam ne verear reformidans. Scaevola expetenda ei vel, sensibus mediocrem dignissim id usu, dictas verear suavitate mei ad. Nec ad definiebas disputando. Debitis habemus alienum in mea, menandri posidonium an mel.

Kapitel 8

Zusammenfassung und Ausblick

8.1 Zusammenfassung

If we summarize what we found, we shall say: That's it. So let's have a close look on all of them.

8.2 Ausblick

Zum Teil ist hiermit schon die Struktur von CdHgTe erforscht worden. Doch noch immer bleiben viele Fragen offen. Zum Beispiel sollte es möglich sein, Kristalle im MBE-Verfahren zu züchten und ihre Struktur in ARPES zu untersuchen.

Des weiteren ist insbesondere der Energiebereich 20 bis 40 eV sehr interessant. An dieser Stelle sollte der Gamma-Punkt liegen. Dispersionsdaten hierzu liegen noch nicht vor.

Kapitel 9

Anhang

9.1 ab initio Berechnungen in einem Supercluster

Die Quelldaten können leicht im Internet gefunden werden. Die Adresse lautet wie folgt ... Es ist leicht zu bedienen, Einige Parameter werden benötigt.

9.2 Datankonvertierung für Analyseprogramme in C++ und Java

Hier ein Beispiel mit GUI (Graphical User Interface). Sehr schon, läuft auch auf einem Mac wegen Qt und C++. Eine ebenfalls plattformunabhängige Version wird in Java mit Javabeans geschrieben. Das .jar file ist dann einfach mit Doppelklick zu öffen und erweckt den Eindruck eines vollständigen Programms.

```
 % Quellcodekopie
// ------------------------------------------------
// vir2qti.cpp
// Konvertierung der WESPHOA Messdaten im
// VIR-Format zu qti fr qtiplot
// Aufruf: vir2qti [quelldatei]
// ------------------------------------------------

#include <iostream>
#include <fstream>
#include <string>
#include <sstream>
#include <iomanip>

using namespace std;

float dataz();
string datas();

char usage[] = "Aufruf: vir2qti [quelldatei]";
bool ok = true;

fstream f;

int main(int argc, char *argv[])
{
  char   ziel[256]   = "",
         quelle[256] = "";
  string linie(60,'-');

{
  char datastrg[256]="";
  float valuez=0;
  if(!f.eof()) { f.getline (datastrg,sizeof(datastrg)); }
  istringstream istr (datastrg);
  istr >> valuez;
  return valuez;
}
string datas()
{
  char text[256]="";
  if(!f.eof()) { f.getline (text,sizeof(text)); }
  if(text == "") { strcpy(text," "); }
  return text;
}
```

9.3 Veröffentlichungen

Eine kleine Liste all jener Veröffentlichungen, an denen ich teilgenommen habe.

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