Determination of the Electronical Bandstructure by Angle Resolved Photoemission

Research Seminar Surface Physics

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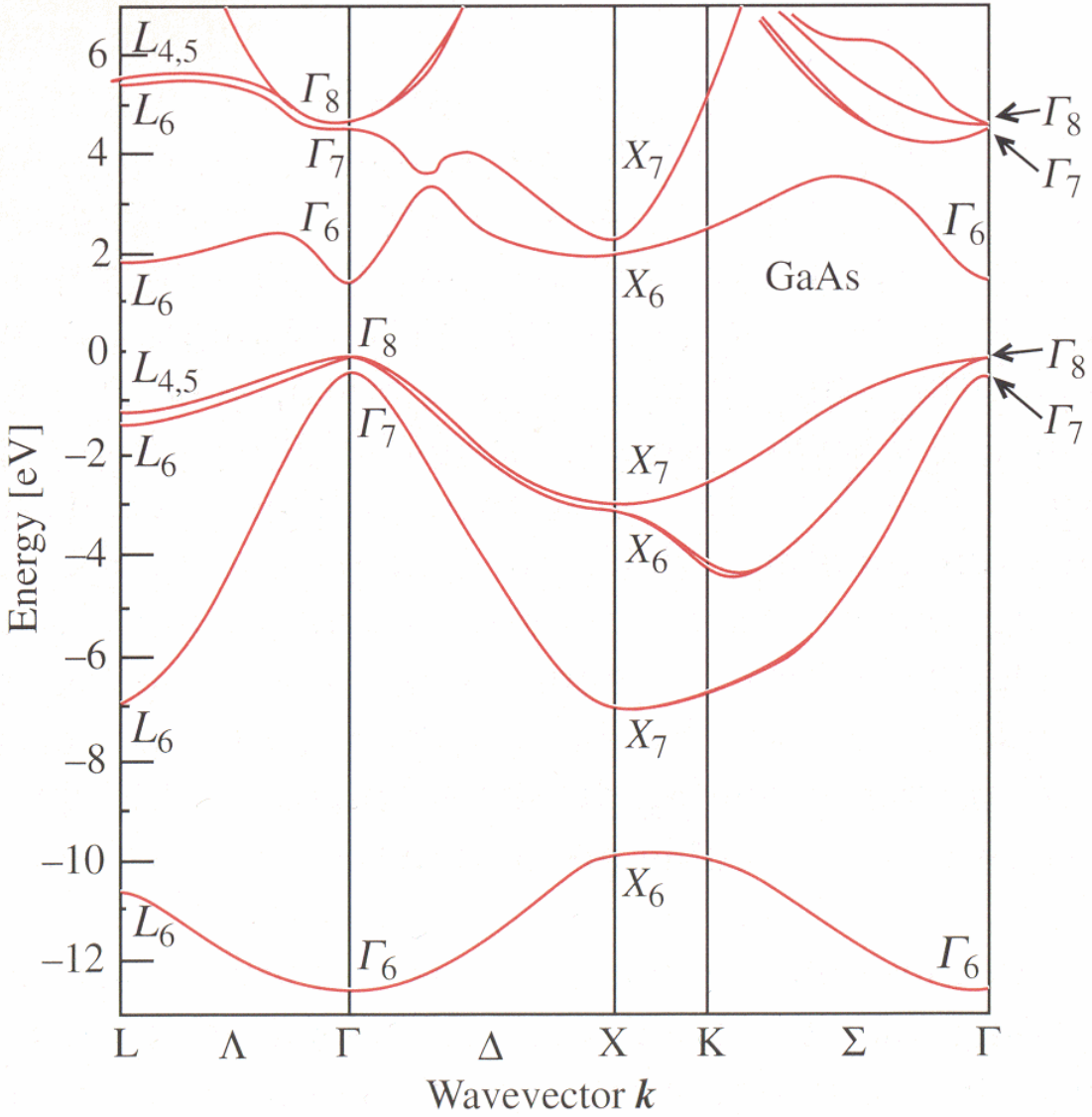
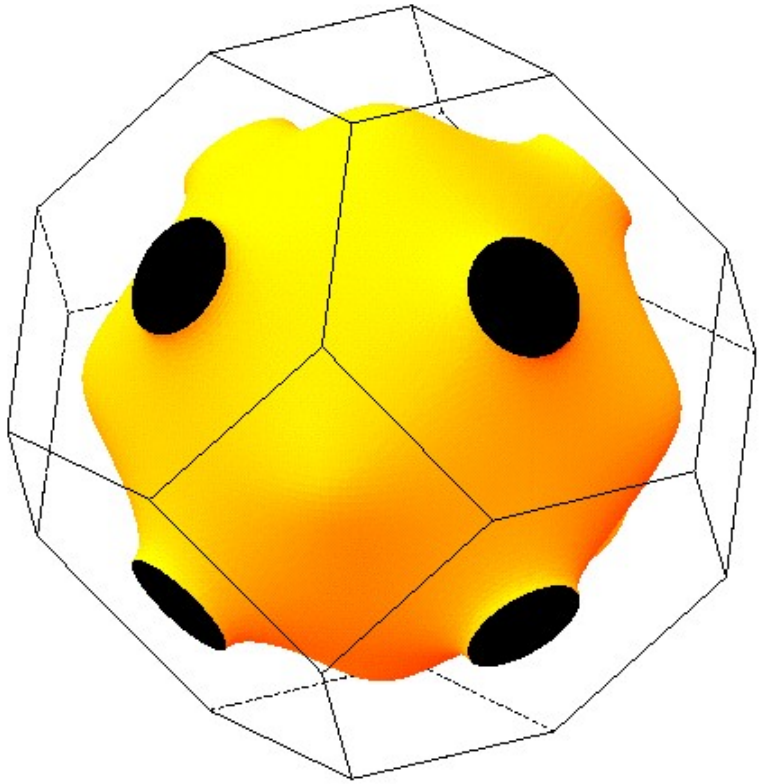
Overview

1. Motivation
2. Angle Resoved Photoelectron Spectroscopy
   - Introduction and Basic Principle
   - Energy Relations and Analysis
   - Design of an Energy Analyser
3. Zero Gap Semiconductor
   - Survey in Gray Tin
   - Alloys of CdTe and HgTe
4. Measurements and Results
   - Preparation
   - Measurement Results
5. Summary and Outlook
   - Summary
   - Outlook

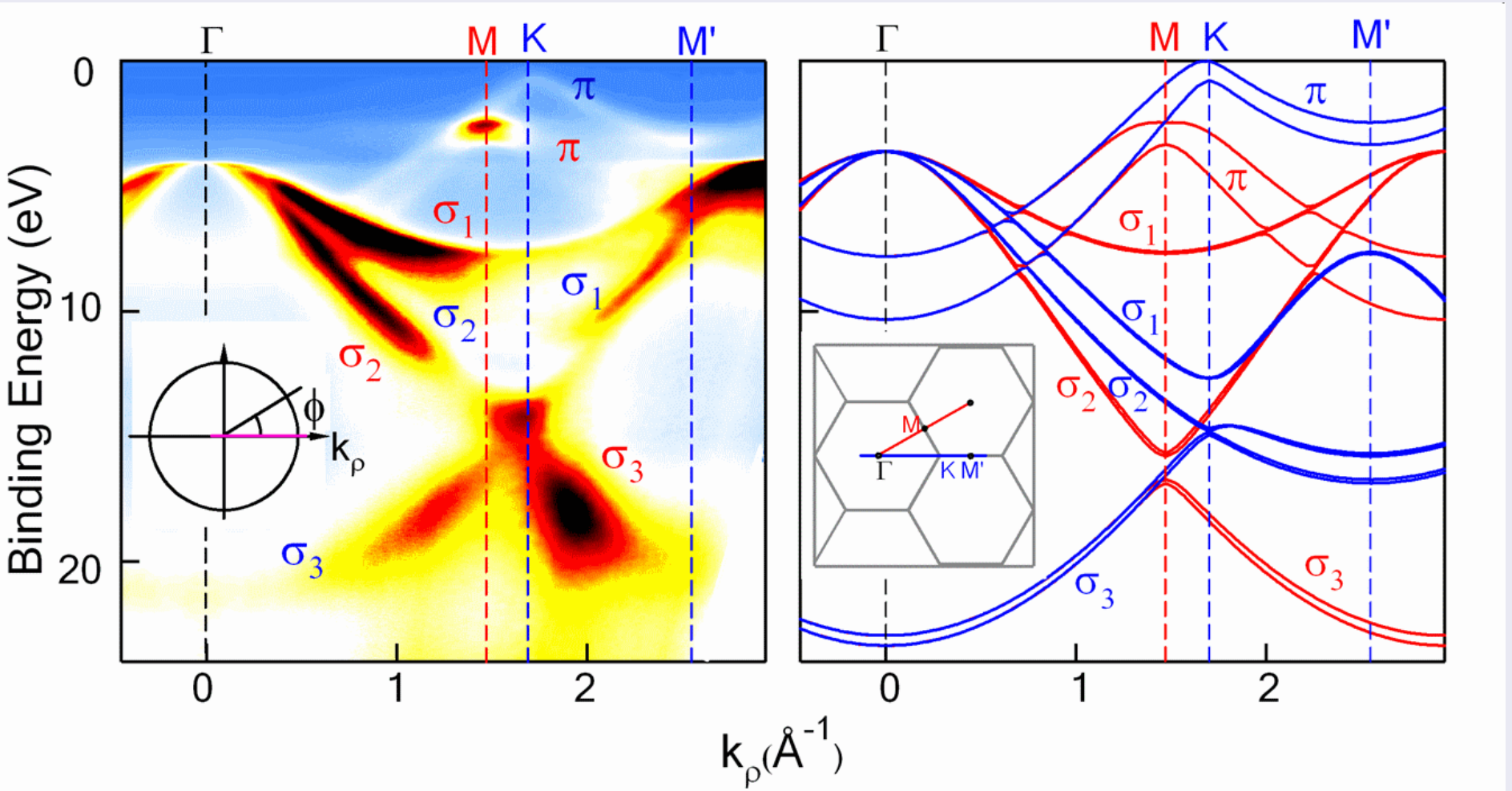
Bandstructure and Fermi Surface



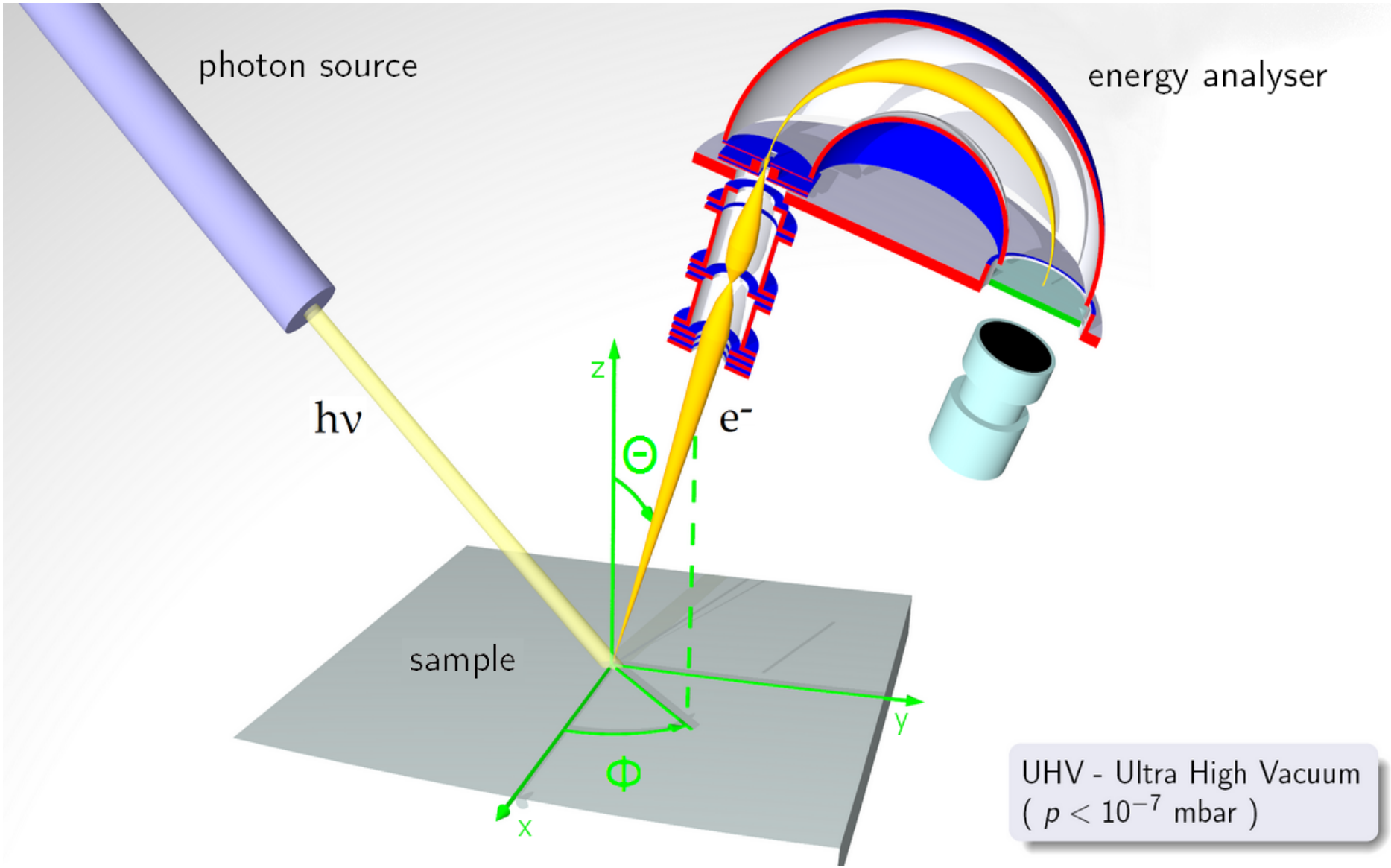


Experimental Results vs. Theory

Photo Electron Spectroscopy on Graphite



General Setup



UHV - Ultra High Vacuum
($p < 10^{-7}$ mbar)

Step 1: Photoexcitation of the Electron

Transition Propability

The probability ω_{fi} of the transition for an electron from initial state $|\Phi_i\rangle$ to final state $|\Phi_f\rangle$ is given by Fermis Golden Rule:

$$\omega_{fi} = \frac{2\pi}{\hbar}|\langle\Phi_f|H_{WW}|\Phi_i\rangle|^2\delta(E_f - E_i - \hbar\omega)$$

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Hamiltonian

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Energy Konservation

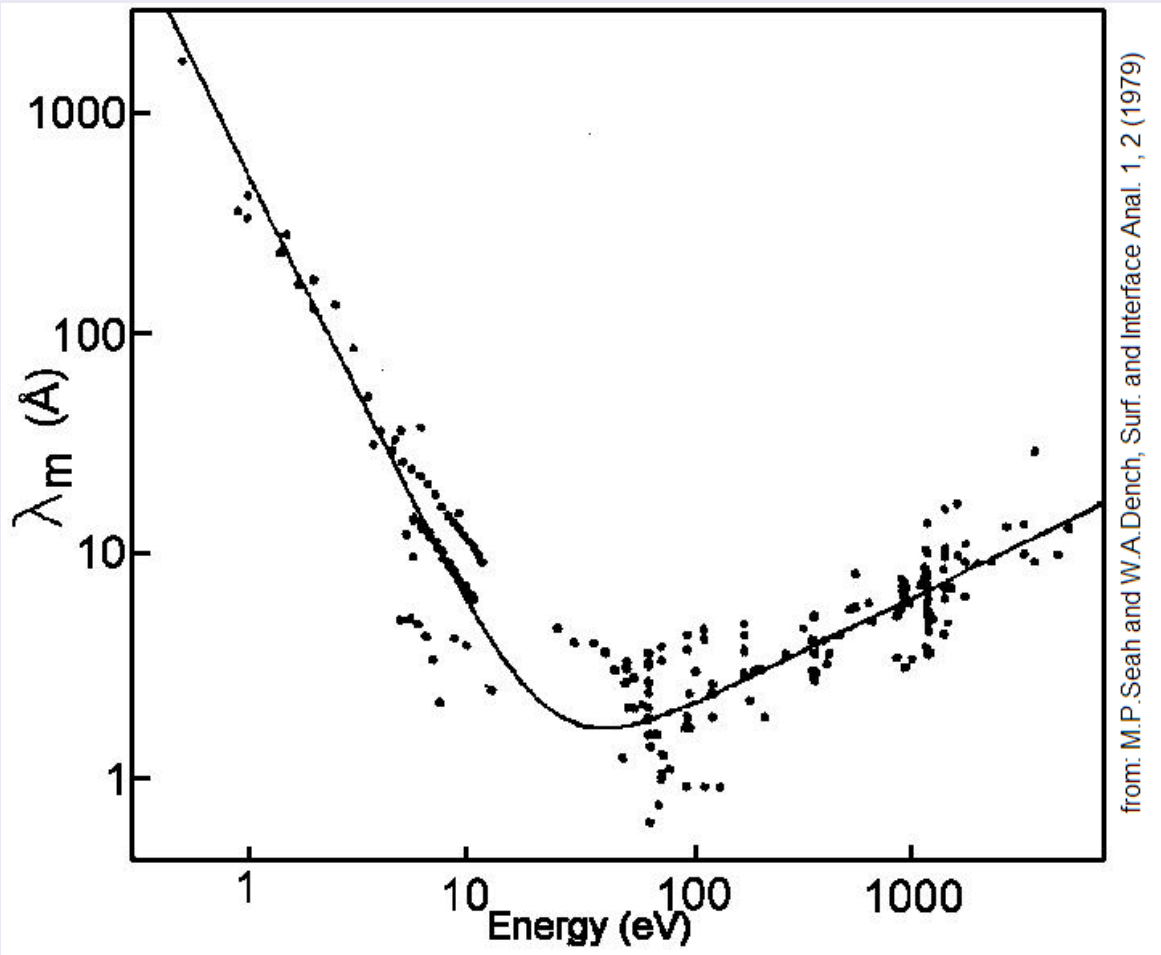
$$E_f = E_i + \hbar\omega$$

Momentum Konservation

$$\vec{k_i} = \vec{k_f}$$

Step 2: Transport to the Surface

Mean Free Electron Path in Bulk Material



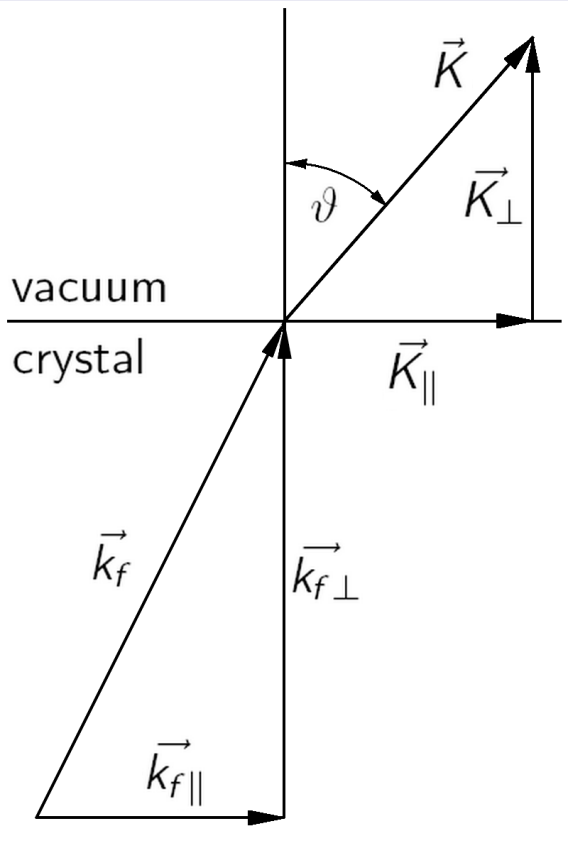
Limiting Step

At UV excitation energies the mean free path is merely 10 Å. One has to care about surface states, clean surfaces that represent bulk material and UHV conditions. Surface sensitivity can be used for band deflection by controlled adsorption.

Secondaries

By scattering a spectra of low energy secondary electrons is generated.

Step 3: Penetration through the surface



$\vec{K}$ wave vector in vakuum, $\vec{k}_f$ is wave vector of the final state in crystal

Dispersion of free Electron

Excited bulk state interacts with free electron state:

$$E_{kin} = \frac{\hbar^2}{2m_e}\vec{K}^2$$

Refraction of Electrons at Surface

Parallel component (plus lattice vector $\vec{g}_\parallel$):

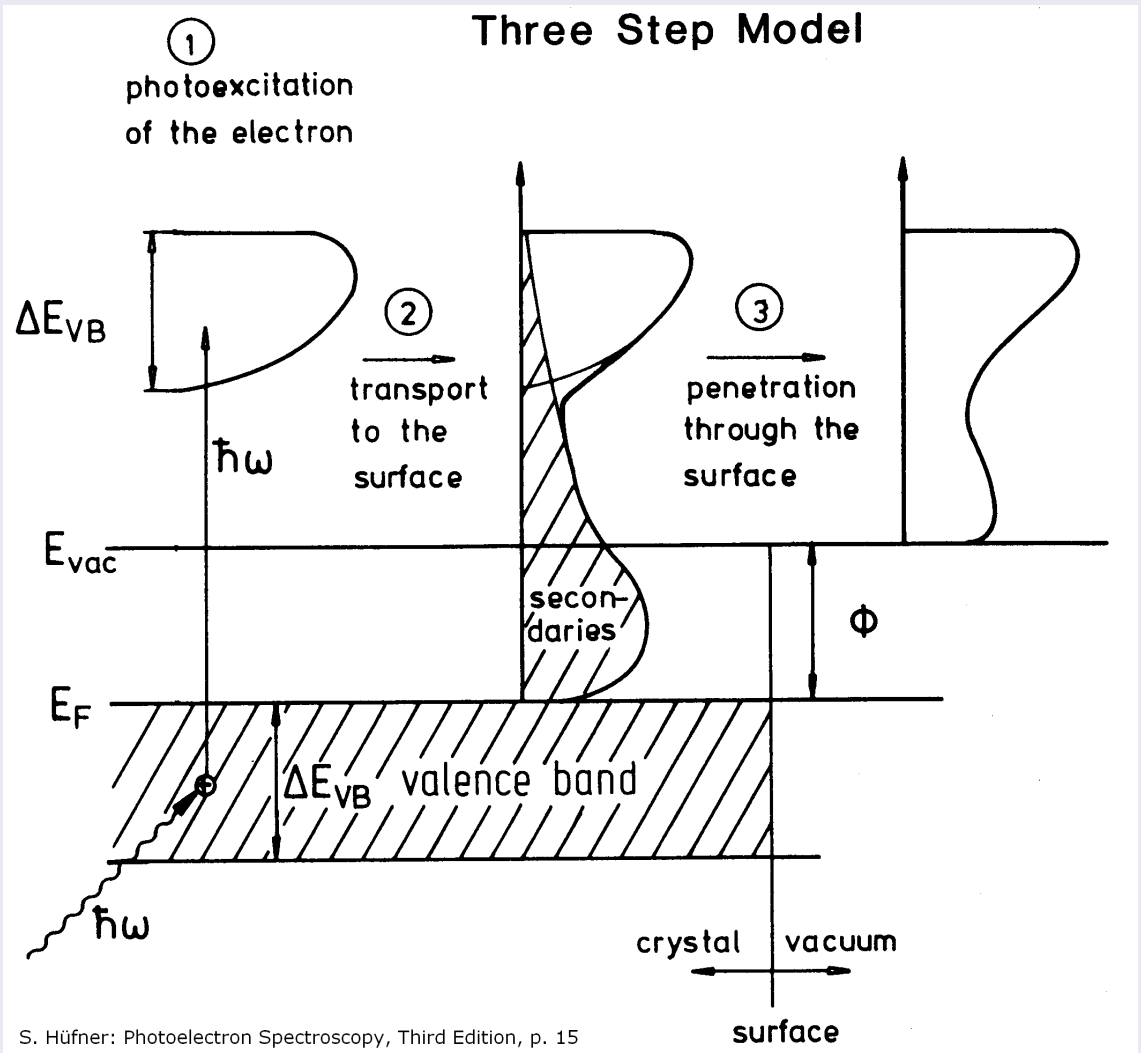
$$\vec{k}_{i_\parallel} = \vec{k}_{f_\parallel} = \vec{K}_\parallel = \sqrt{\frac{2m}{\hbar}E_{kin}}\sin\vartheta$$

Final state energy and perpendicular component:

$$E_f = \frac{\hbar^2}{2m}(\vec{k}_f + \vec{G})^2 - |V_0|$$

$$k_{f_\perp} = \sqrt{\frac{2m}{\hbar^2}(E_{kin} + |V_0|) - \vec{G}_\parallel^2} - G_\perp \qquad \vartheta = 0$$

Energy Relations during Measuring Process



S. Hüfner: Photoelectron Spectroscopy, Third Edition, p. 15

Kinetic Energy

$$E_{kin} = \frac{\vec{p}^2}{2m_e} = \frac{m_e}{2}\vec{v}^2$$

Lorentz Force

$$\vec{F} = q(\vec{E} + \vec{v} \times \vec{B})$$

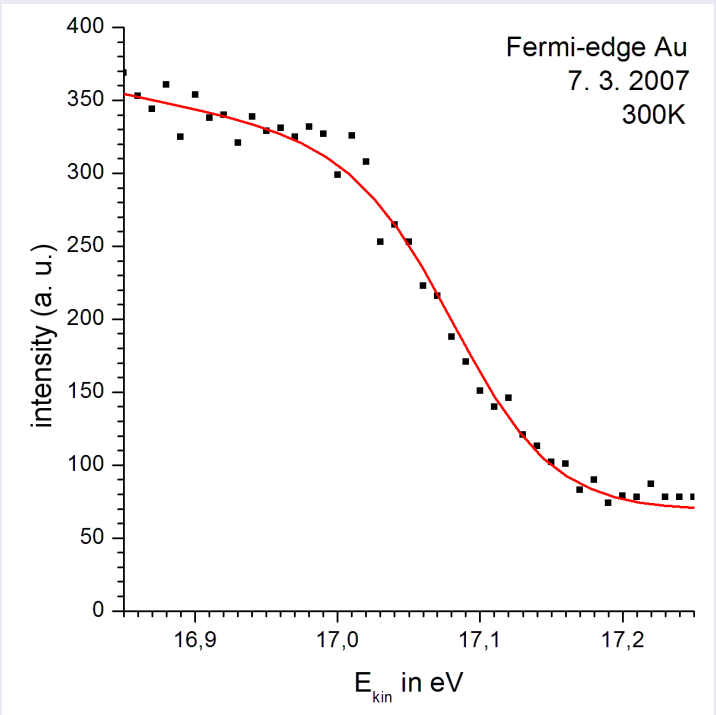
$$\mathbf{B} \leq 0.25\mu T$$

Example

$\hbar\omega$	=	21.2eV	He-I
Φ	=	4.8eV	Au
E_{kin}	=	16.4eV	E_F

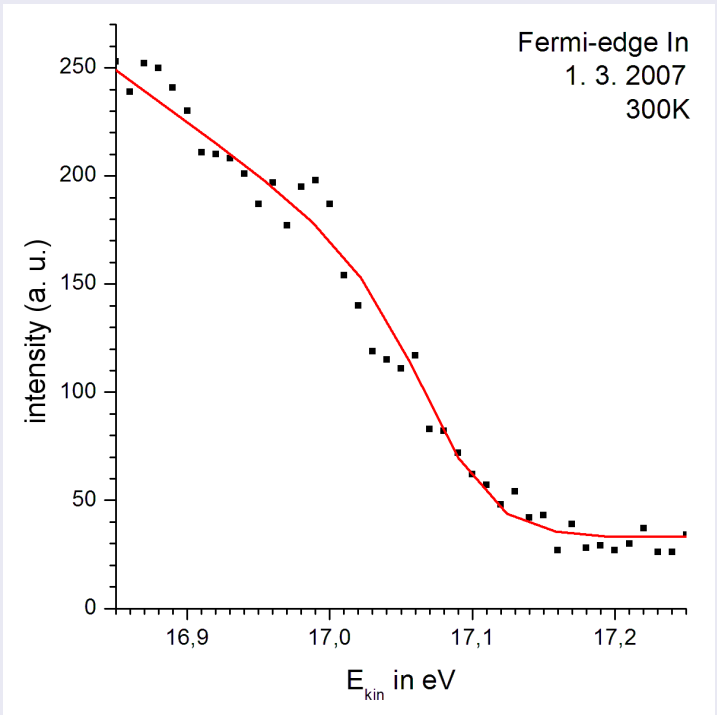
Invariance of measured Fermi-Energy on Work Function

Fermi-edge Gold, $\Phi = 4.8$ eV



$E_F = (17.085 \pm 0.004)$ eV

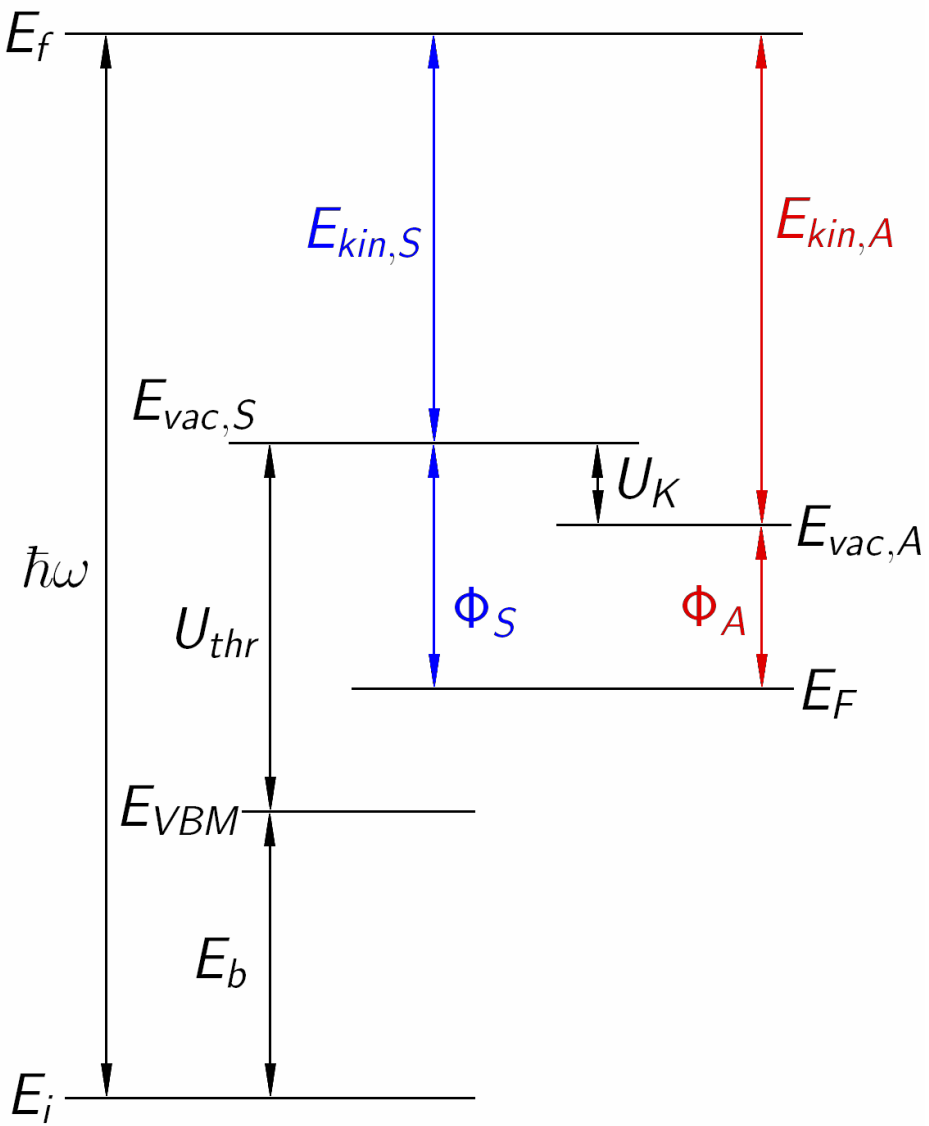
Fermi-edge Indium, $\Phi = 4.12$ eV



$E_F = (17.076 \pm 0.005)$ eV

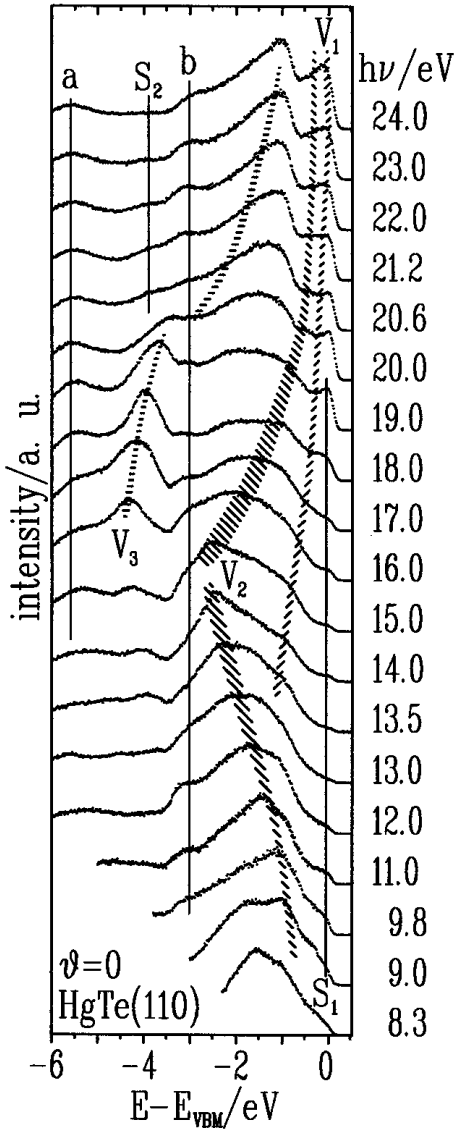
The measured Fermi-energy does not depend on the work function of the sample. During the measuring process the entire spectrum is shifted.

Work Function and Energy Relations



E_i	energy of initial state
E_f	energy of final state
E_{VBM}	valence band maximum
$E_{vac,S}$	vacuum level of sample
$E_{vac,A}$	vacuum level of analyser
$\hbar\omega$	photon energy
U_b	binding energy
E_{thr}	threshold of photo emission
$E_{kin,S}$	kinetic energy of eletrons at the sample
$E_{kin,A}$	kinetic energy of eletrons at analyser
U_K	contact potential
Φ_S	work function of sample
Φ_A	work function of analyser
E_F	Fermi energy

Fitting and resulting Band Structure



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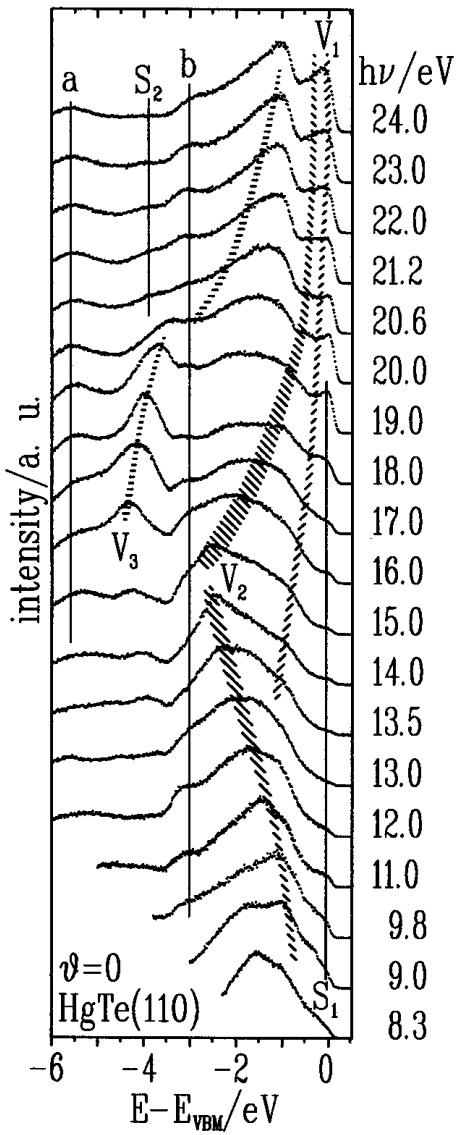
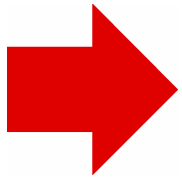
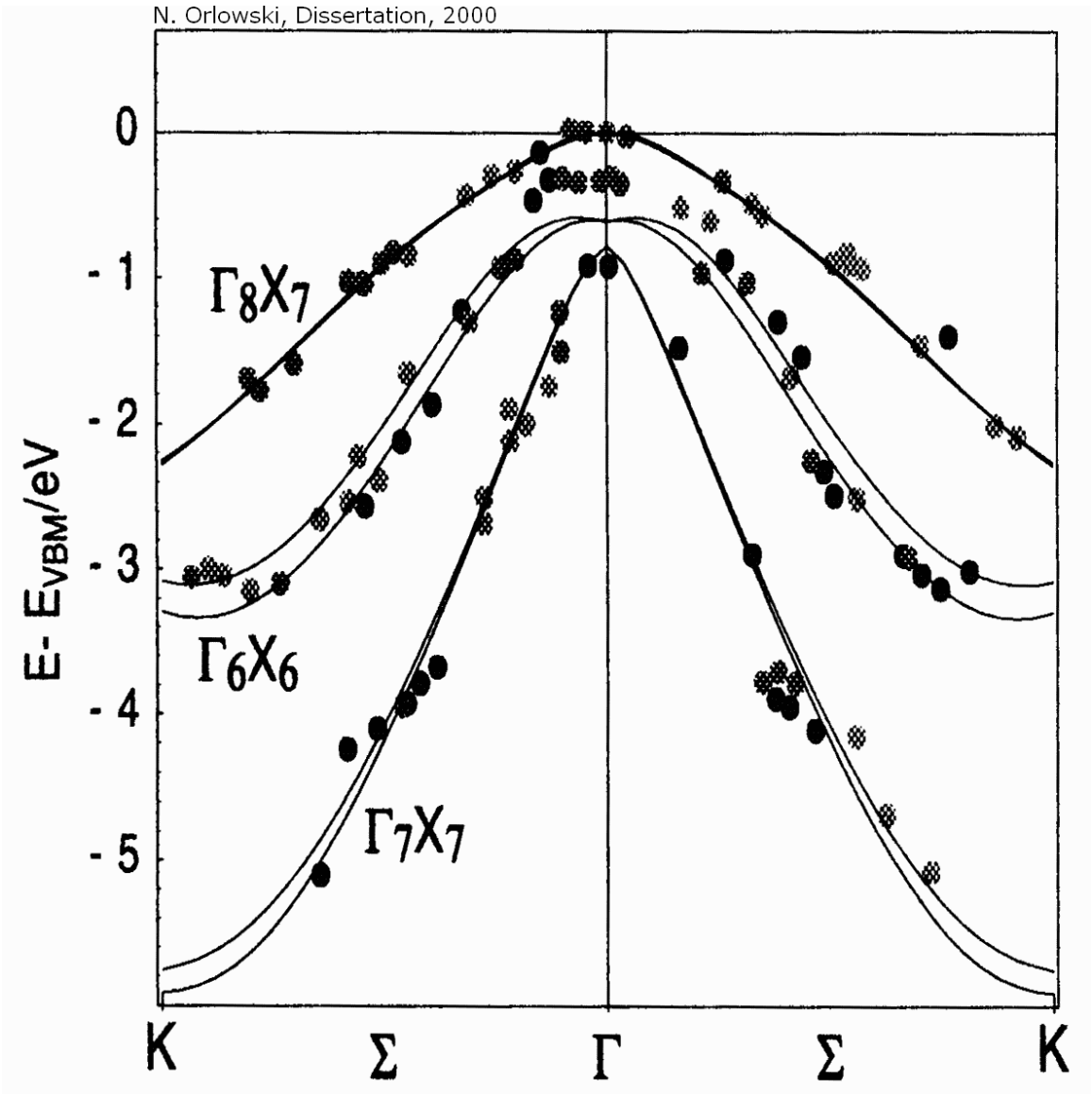
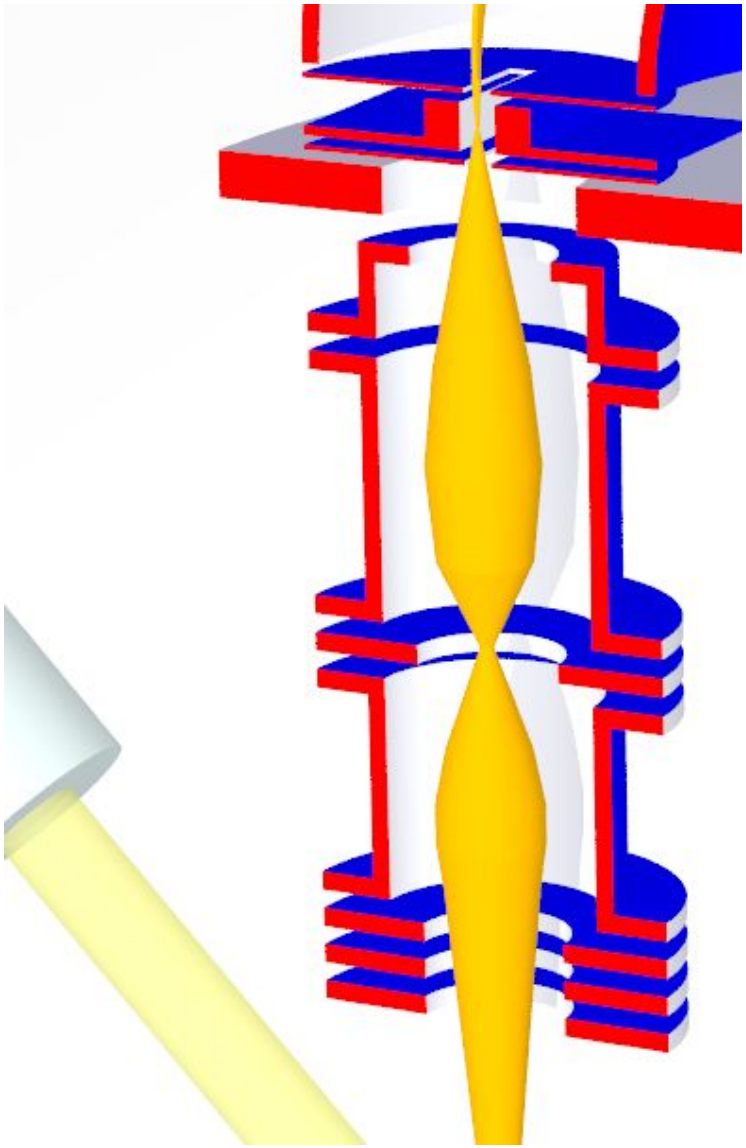






Retarding and Focussing



Preretarding stage

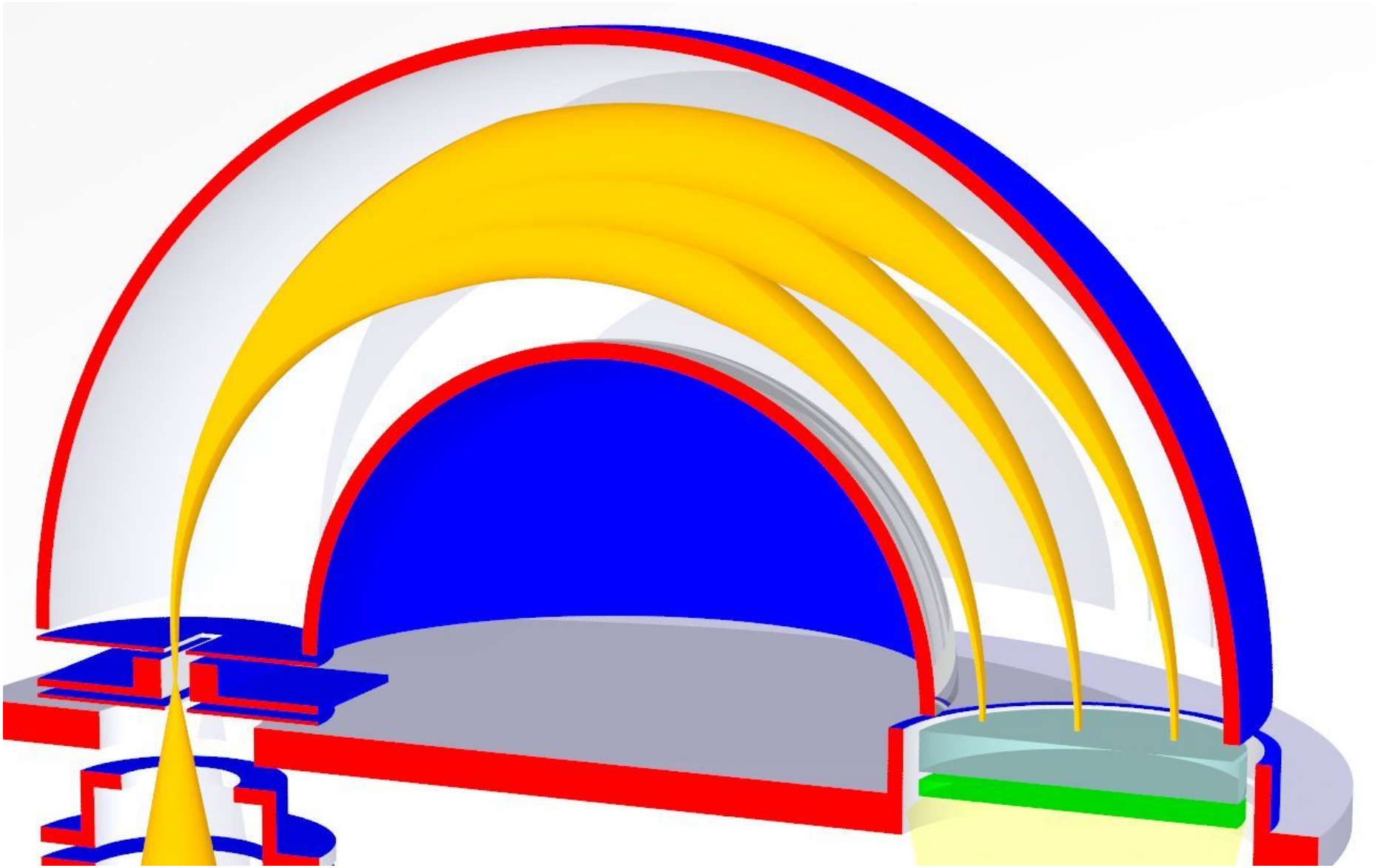
Usually a preretarding stage is used prior to the energy analysis. Electrons enter the analyser with a specified pass energy. One can decelerate (or accelerate) electrons (almost) without changing their absolute energy spread. Measured kinetic energy:

$$E_{kin,A} = E_{pass} - U_{ret}$$

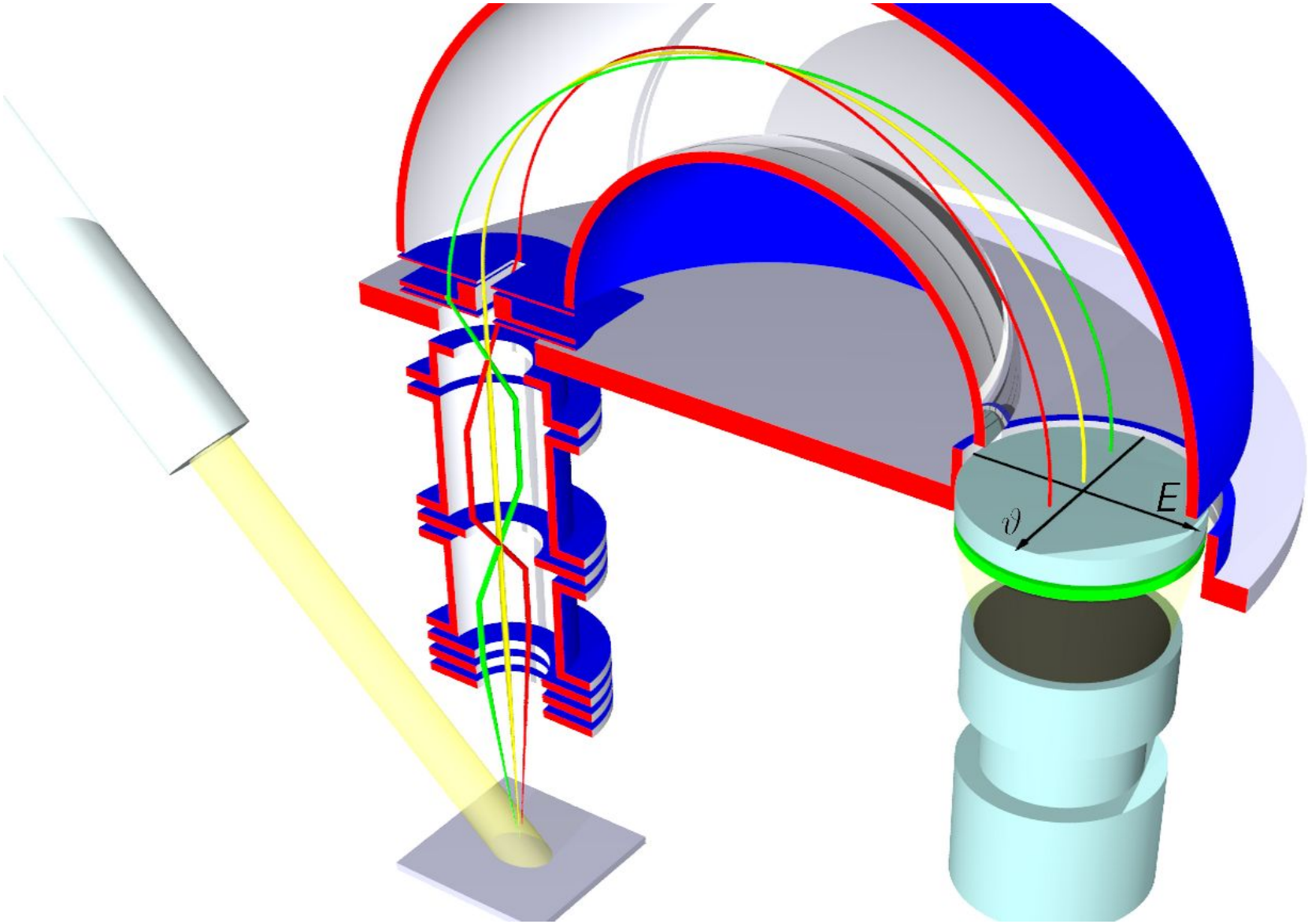
Negative Kinetic Energy

$E_{kin,S}$	=	0.2 eV
U_{ret}	=	10.2 eV
U_K	=	-0.4 eV
E_{pass}	=	10 eV
$E_{kin,A}$	=	-0.2 eV

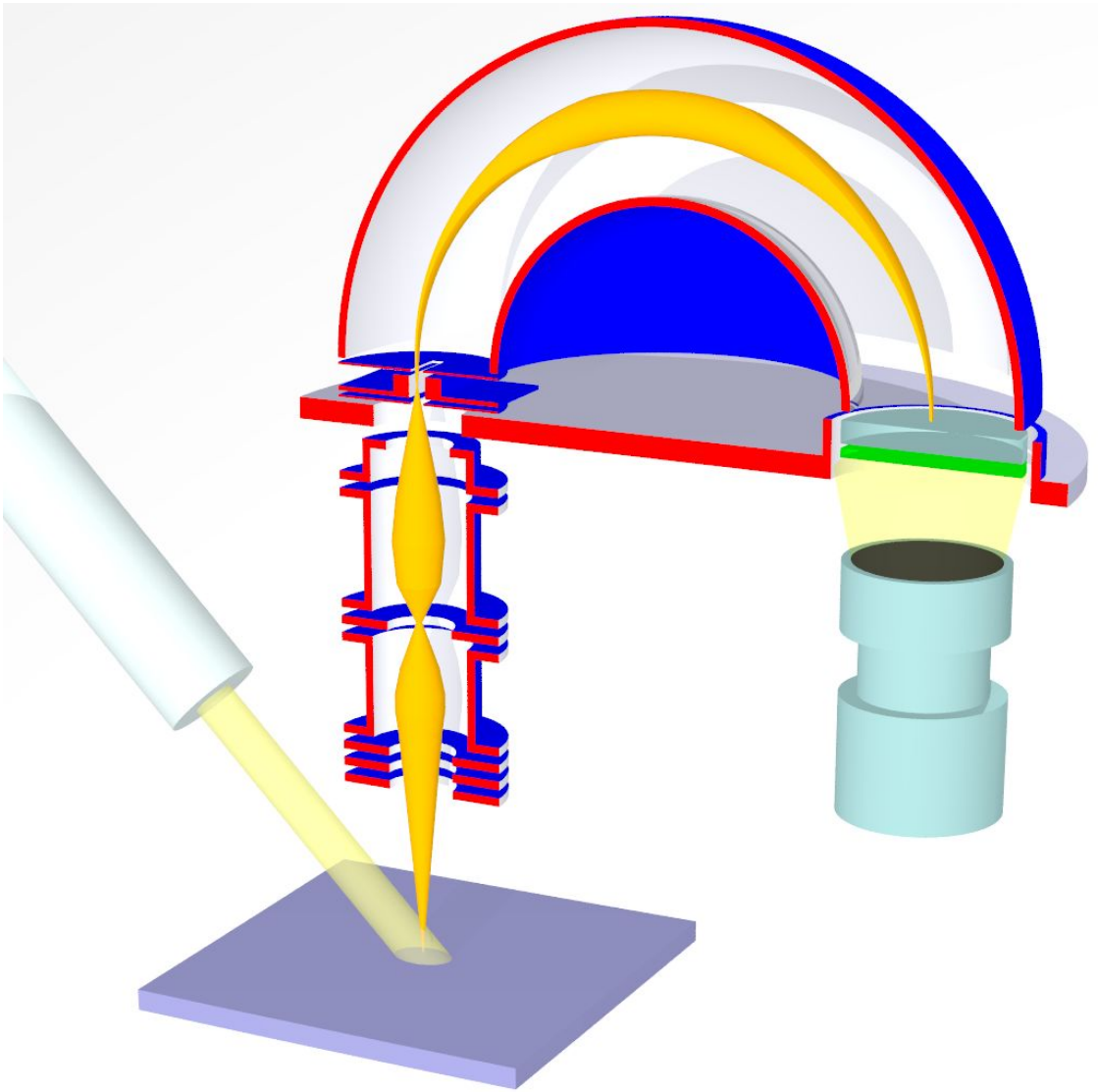
Energy Dispersion inside Spherical Condensator



Angle Resolution by Mapping of Entrance Point



Resolution of Spherical Analyser



Potentials on hemispheres

For transmission of electrons with initial emergy E_0 along a path with $R_0 = (R_{in} + R_{out})/2$ the potential has to be

$$V_{out} = E_0[3 - 2(R_0/R_{out})]$$

$$V_{in} = E_0[3 - 2(R_0/R_{in})]$$

Resolution

$$\frac{\Delta E}{E_{pass}} = \frac{w}{2R_0} + \alpha^2$$

w	width entrance slit
α	acceptance angle

Survey of Narrow-Gap Semiconductors: α-Sn

(I) cruical magnetoresistance measurements on n-type material by Ewald's group which showed no anisotropy at 4 or 77 K but a dominance of electrons of (111) symmetry at 200 K

(II) measurements of conductivity, Hall effect and susceptibility at temperatures above 150 K, which demonstrated an activation energy of 0.08 eV

(III) measurement of an electron mass of 0.02 m_0 which was inconsistent with a small $(\Gamma_8^+ - \Gamma_7^-)$ gap

(IV) pressure measurements which gave a high-temperature pressure coefficient consistens with conduction band minima at the L point

(V) pressure measurements on conductivity and Hall effect at low temperatures which were inconsistent with the presence of (111) electrons and also of (000) electrons in a Γ_7^- *extremum*

No conventional positive-gap band structure could fit all of these criteria.

William Paul & Steven Groves: *Band Structure of Gray Tin*, 1963, Phys. Rev. Lett. **11** 194

Inverted Bandstructure

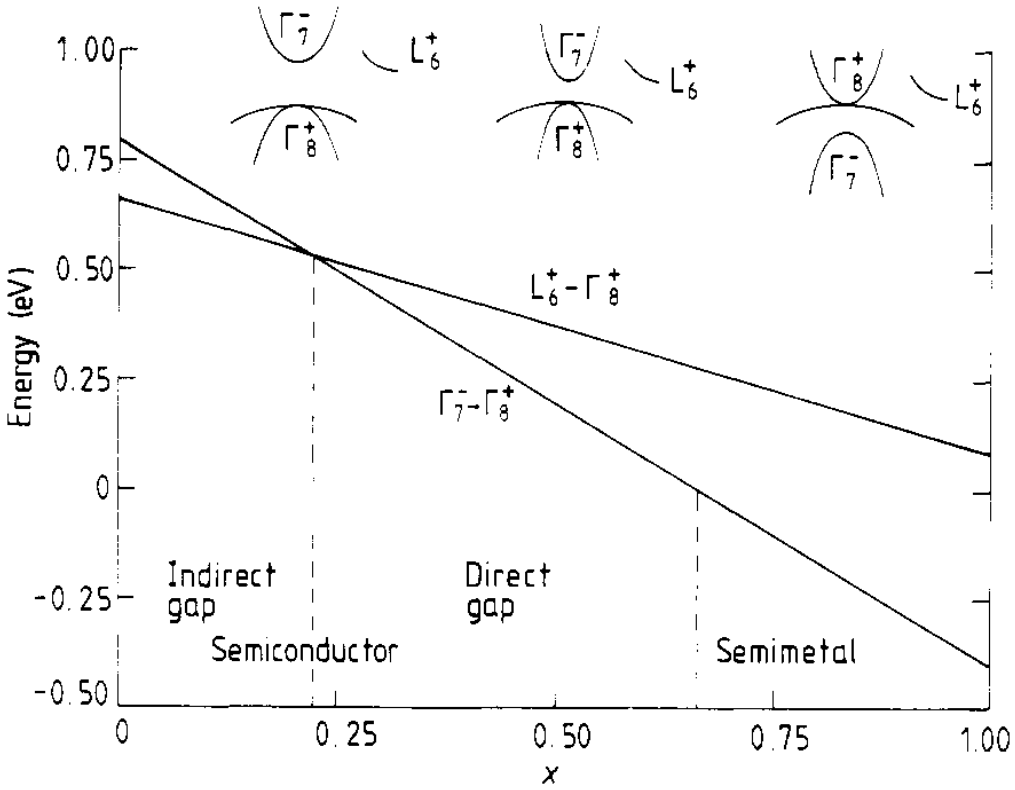


Figure 1. Variation of the energy differences ($\Gamma_7^- - \Gamma_8^+$) and ($L_6^+ - \Gamma_8^+$) in the alloy system $Ge_{1-x}Sn_x$. For $x = 0$, the smallest band gap ($L_6^+ - \Gamma_8^+$) is indirect, with a value of about 0.65 eV at room temperature; the direct gap ($\Gamma_7^- - \Gamma_8^+$) is about 0.8 eV. For $x = 1$, the indirect gap ($L_6^+ - \Gamma_8^+$) is $\sim$ 0.1 eV and the direct gap ($\Gamma_7^- - \Gamma_8^+$) about -0.4 eV.

α-Sn paper

Results for HgTe was in S. Groves thesis, but statement about it was taken out of *PRL* paper in case speculations on this material they had not measured themselves would jeopardise publication.

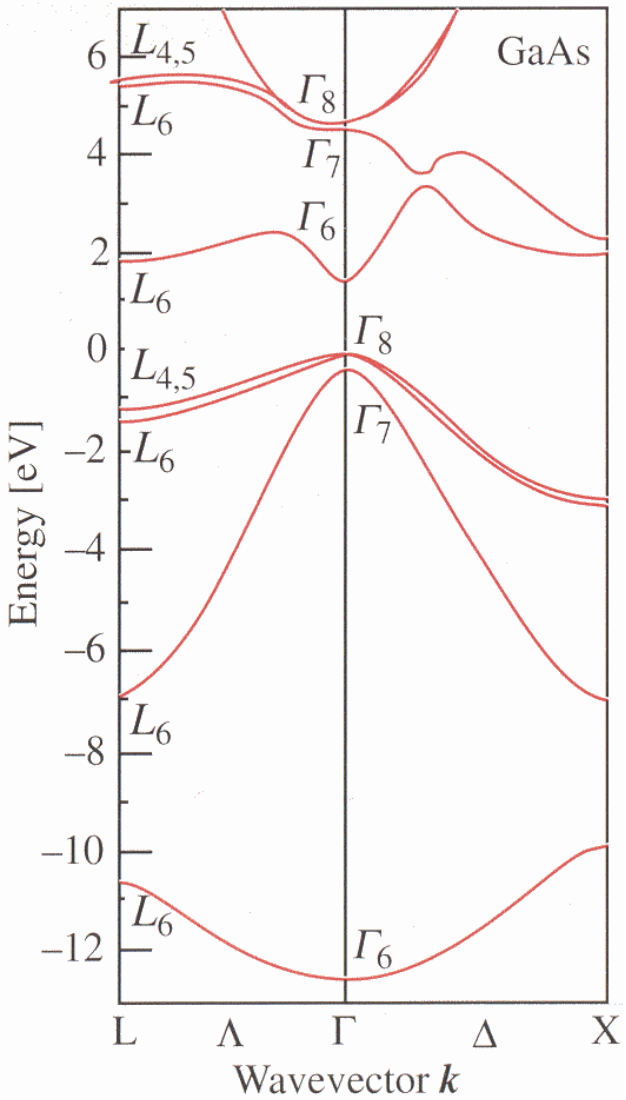
ZnS semiconductors

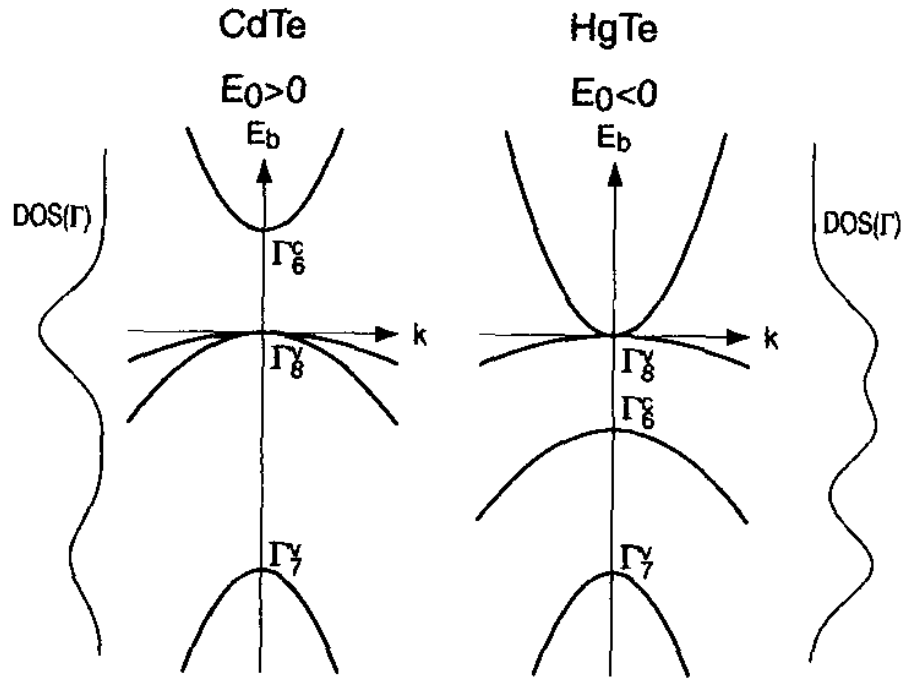
bandgap definition:

$$E_0 = E(\Gamma_6) - E(\Gamma_8)$$

(direct bandgap)

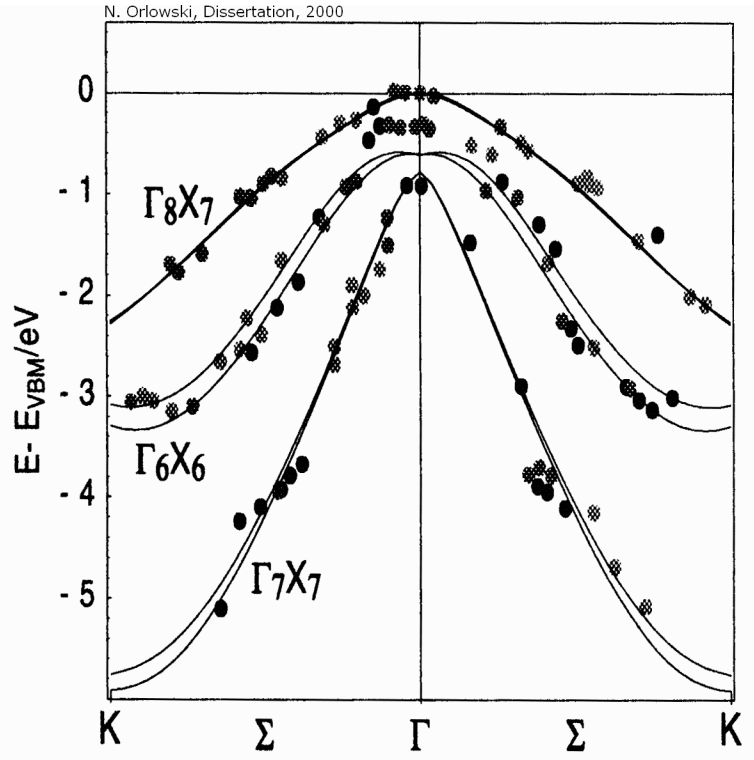
Bandgap for $CdTe$, $HgTe$ and $Cd_xHg_{1-x}Te$





CdTe	property	HgTe
0,675	Phillips-Van Vechten ionicity f_i	0,68
6.488	lattice constant	6.445
1.56	gap	-0.283

$Cd_xHg_{1-x}Te$



inverted bandstructure of HgTe, measured with ARPES

Properties

CdTe and HgTe are consolute. The bandgap can be free adjusted. The alloys have a high electron mobility and a high optic absorption coefficient.

Fabrication

- modified Bridgeman technique
- molecular beam epitaxy (MBE)

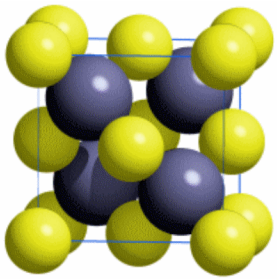
Application

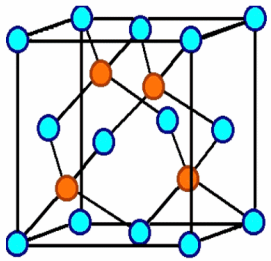
- dual-band infrared detectors with high quantum efficiency (simultaneous detection in the MWIR and LWIR)
- CCD-array for IR-astronomy

Samples of $Cd_xHg_{1-x}Te$

Data of Samples

Nr.	X	weight
Ia	0,07	127 mg
Ib	0,07	
II	0,4	130 mg
IIIa	0,2	92 mg
IIIb	0,2	67 mg
IV	0,183	129 mg
V	0,1955	248 mg
VI	0,105	109 mg





Crystal Quality - Laue Images

Polaroid and Simulation

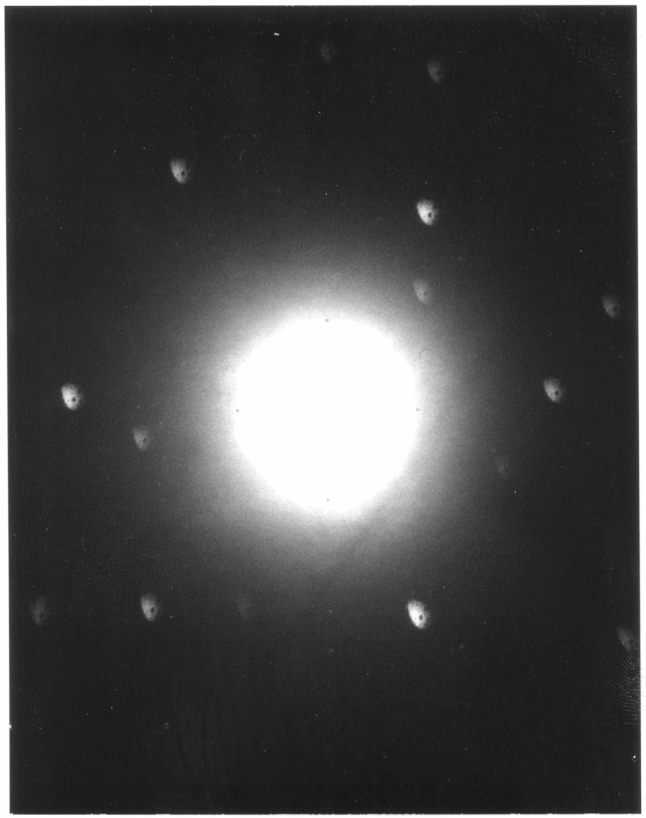


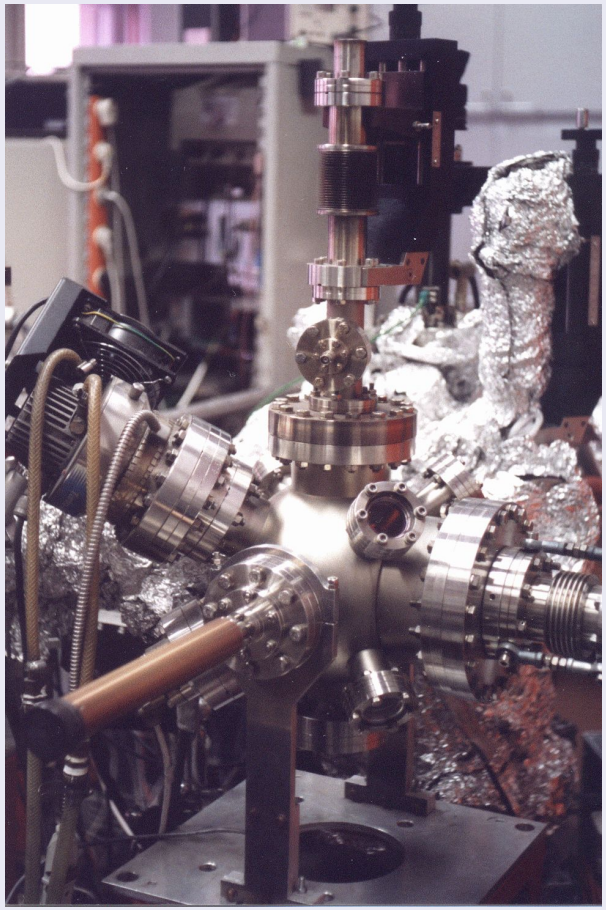
image generated with LauePT 2.1 (programm for Laue Pattern, programmed by XianRong Huang, Stony Brook University, Southhampton; www.sunysb.edu)

Sample Ib

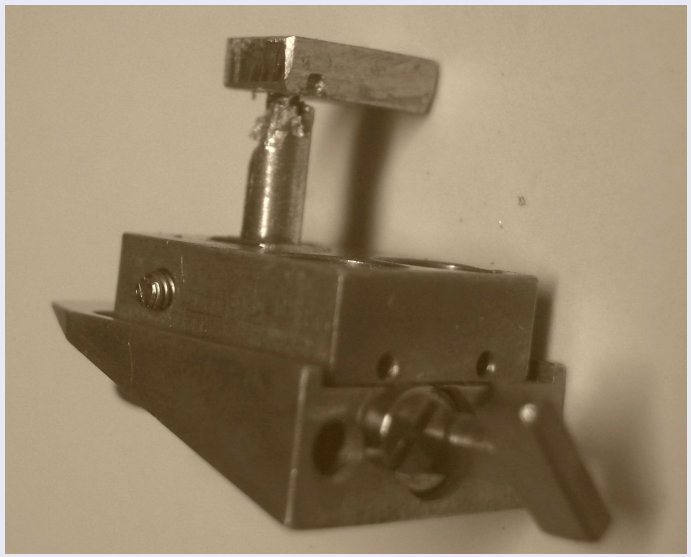
$Cd_{0.07}Hg_{0.93}Te$

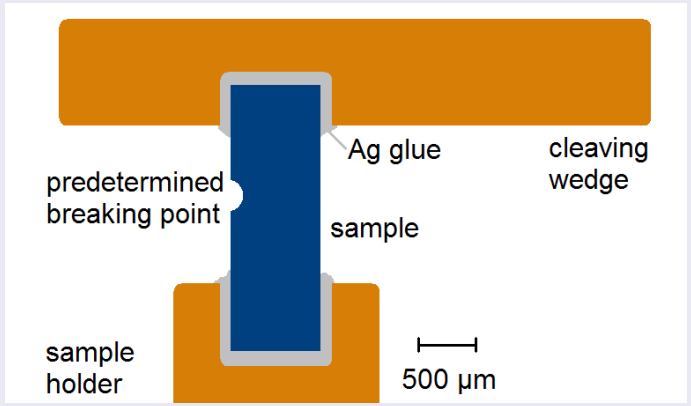
thickness: 620 μm
weight: 81 mg

Surface Preparation - Cleavage Mechanism



cleavage chamber by
N. Orlowski, assembled 2000

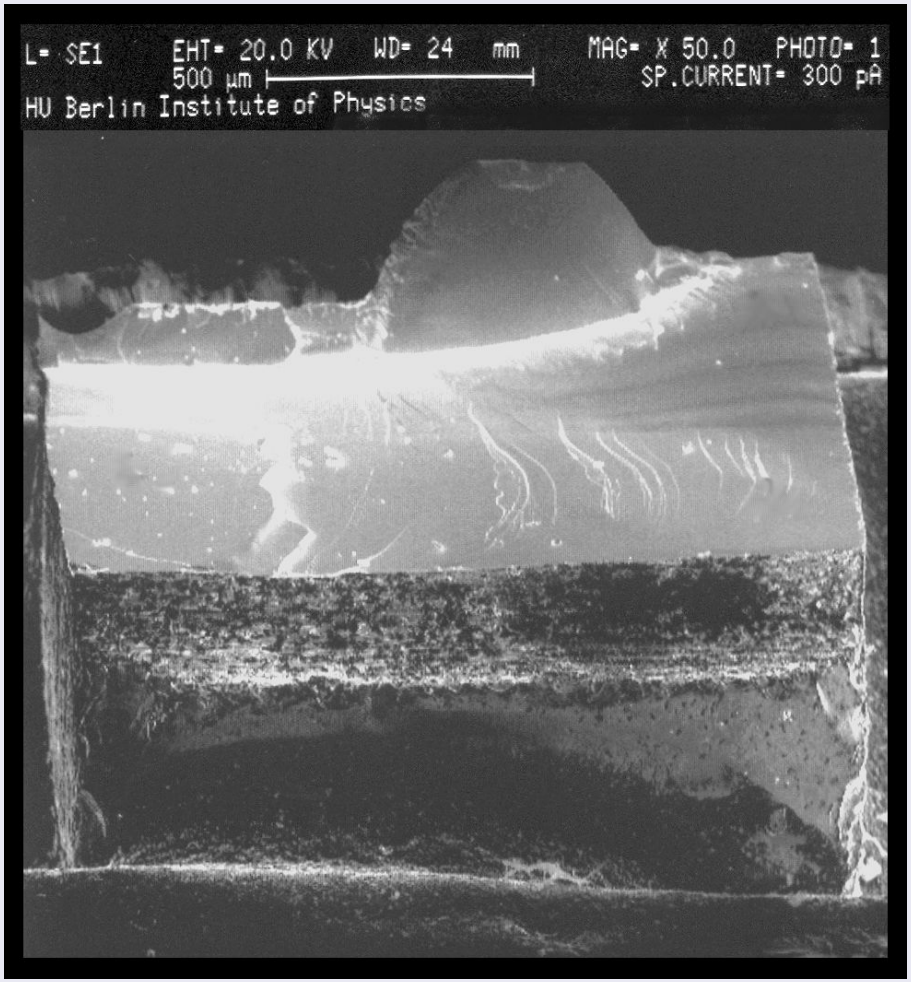




cleavage in sample holder

Surface Quality after Cleavage

SEM Image

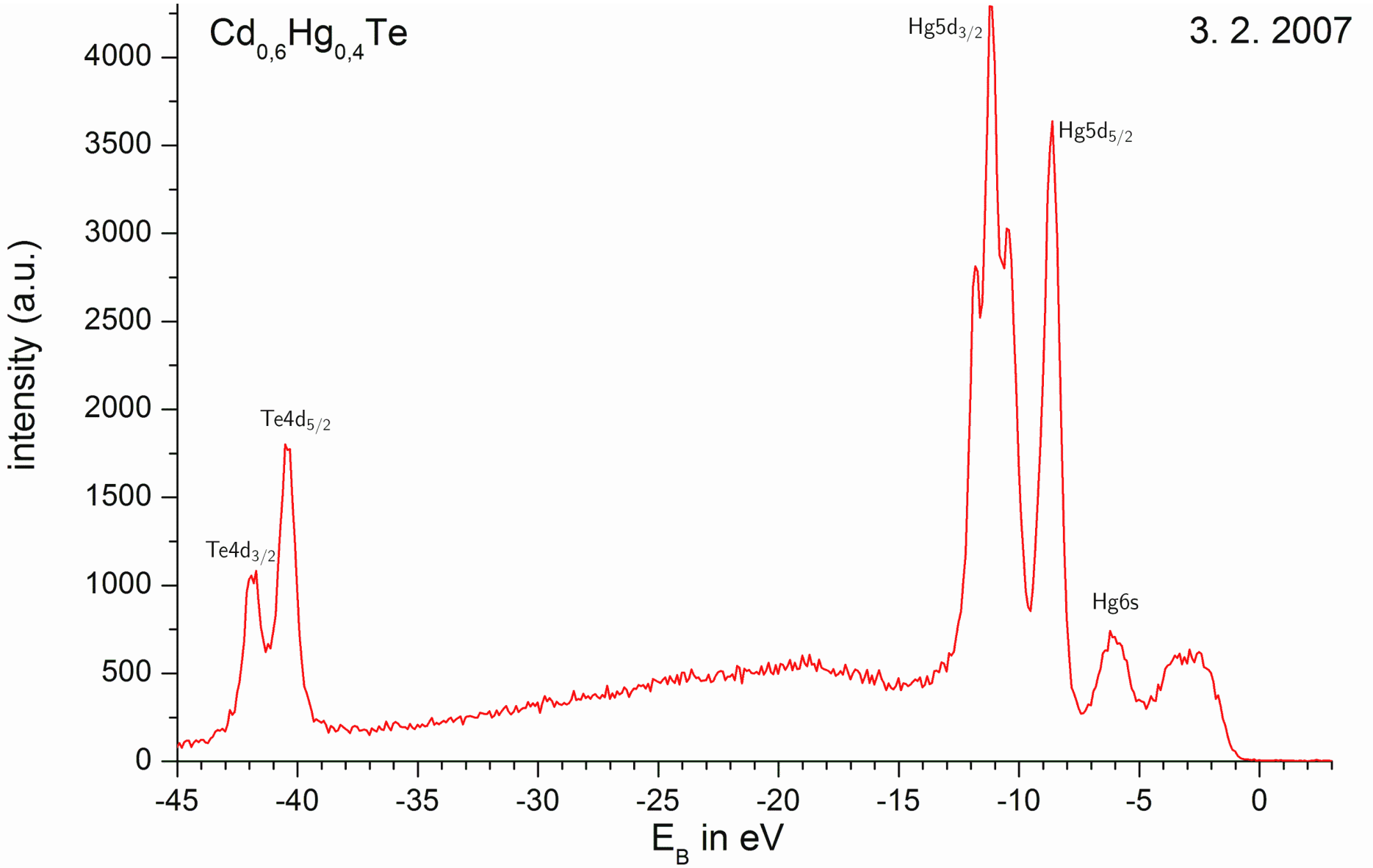


LEED Image

Reasons for LEED

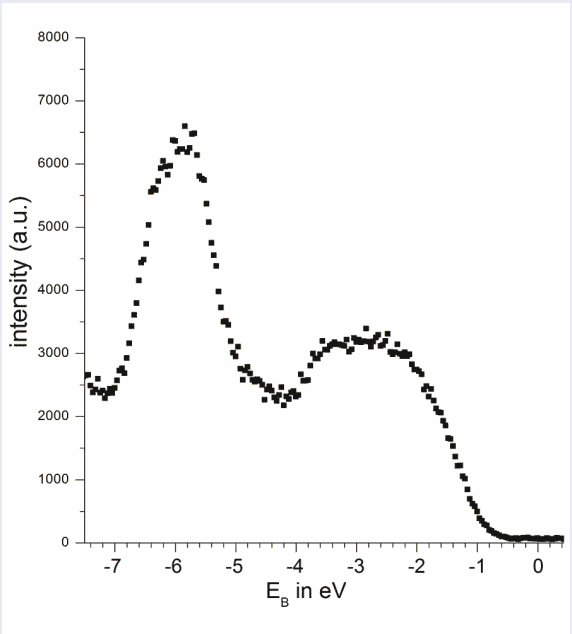
- craggedness of cleavage
- spot size electron beam
- failure in apparature

BESSY Measurements at BUS Beamline, $\hbar\omega = 80$ eV



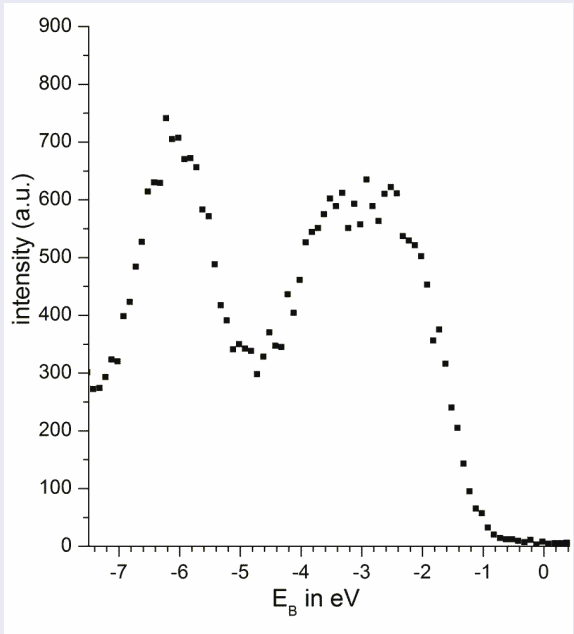
Dispersion in Valence Band? Gap? Peak Position?

BESSY $h\nu = 40$ eV



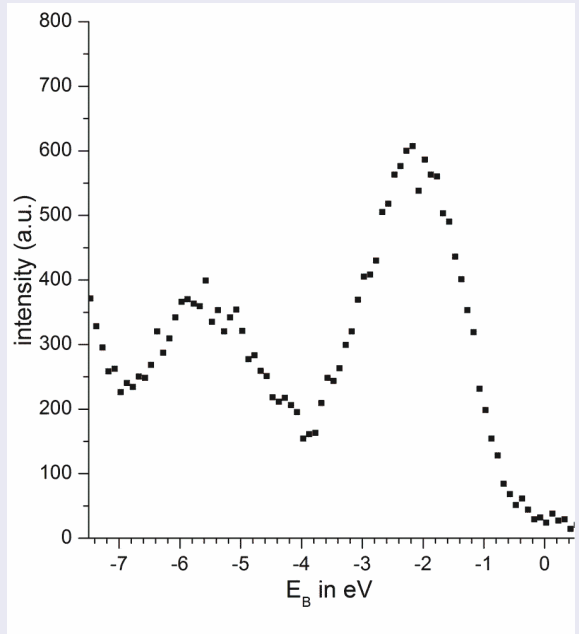
$Cd_{0.18}Hg_{0.82}Te$
26. 1. 2007

BESSY $h\nu = 80$ eV



$Cd_{0.4}Hg_{0.6}Te$
3. 2. 2007

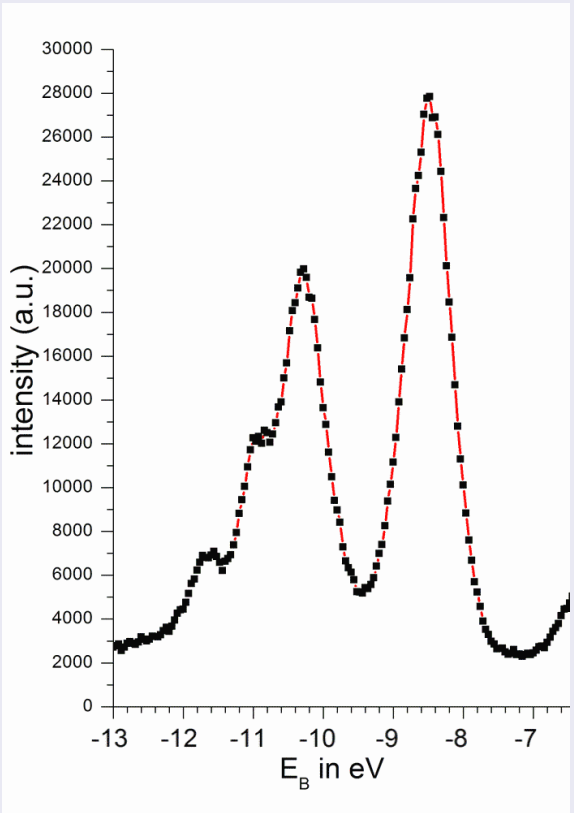
He-I $h\nu = 21.2$ eV



$Cd_{0.2}Hg_{0.8}Te$
8. 3. 2007

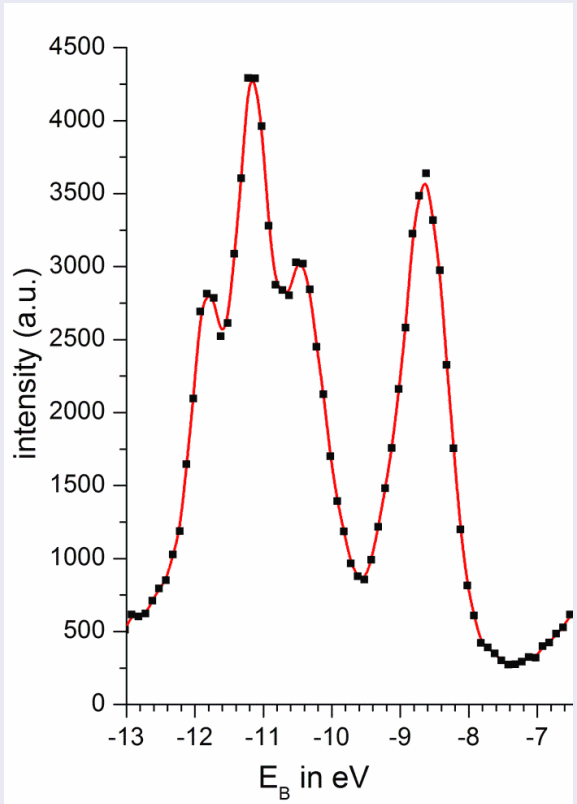
Cleavage Quality - Satellites of $Hg5d_{3/2}$

BESSY $h\nu = 40$ eV



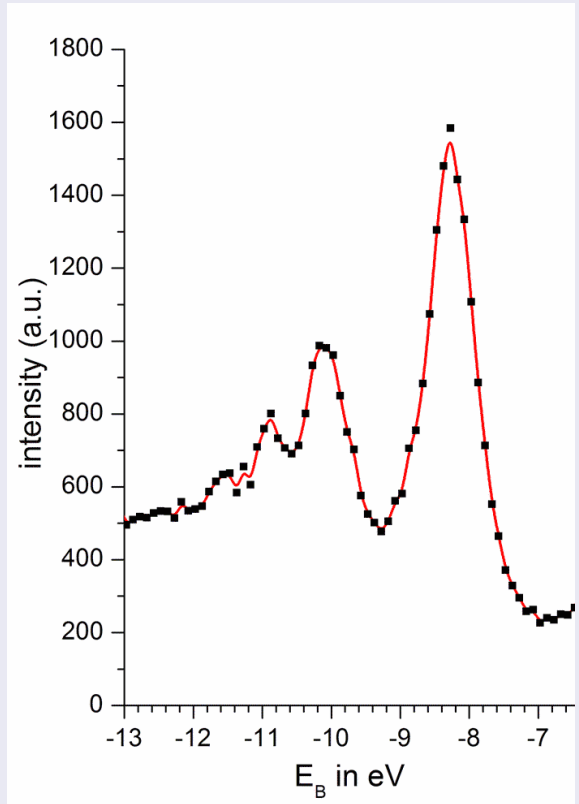
$Cd_{0.18}Hg_{0.82}Te$
26. 1. 2007

BESSY $h\nu = 80$ eV



$Cd_{0.4}Hg_{0.6}Te$
3. 2. 2007

He-I $h\nu = 21.2$ eV



$Cd_{0.2}Hg_{0.8}Te$
8. 3. 2007

X. Yu, L. Vanzetti, G. Haugstad, A. Raisanen, A. Franciosi: *Inequivalent sites for Hg at the HgTe (110) surface*. Surf. Sci **275**, 92-100, (1992)

Conclusion

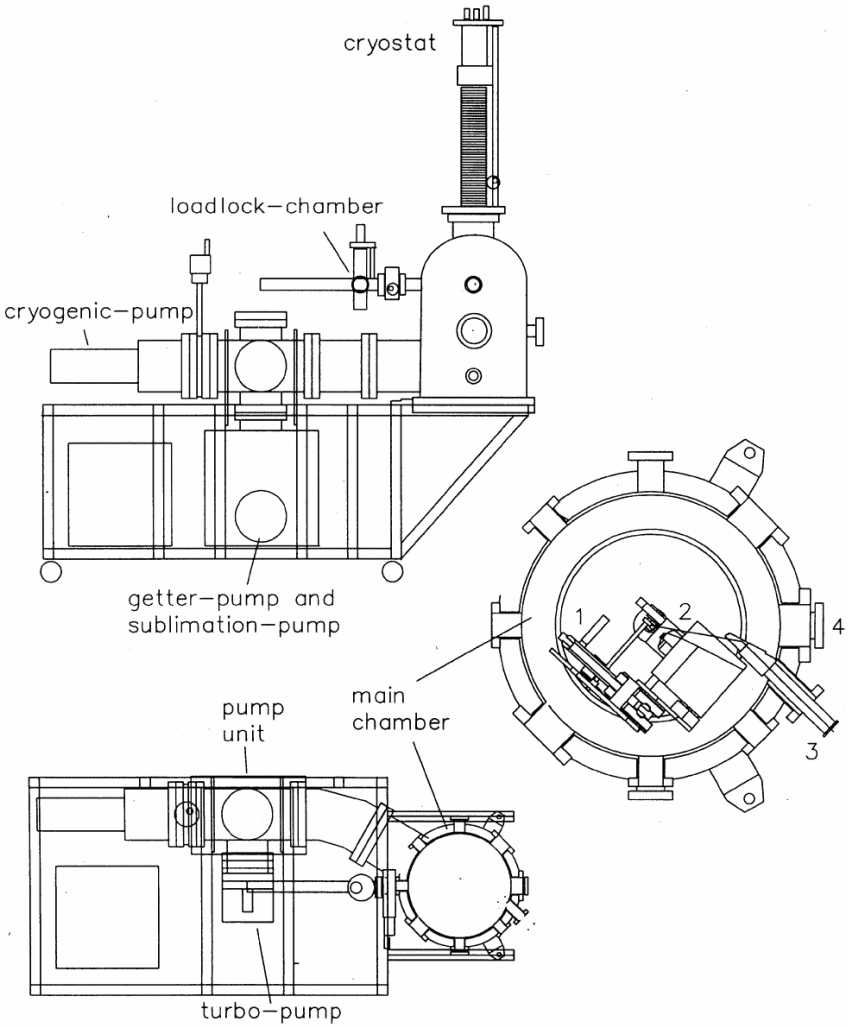


Photo Electron Spectrosopy

- powerfull technique to determine bandstructure and electronic properties of solids
- detected electrons easy to analyse
- surface sensitive
- UHV conditions inevitable

Conclusion

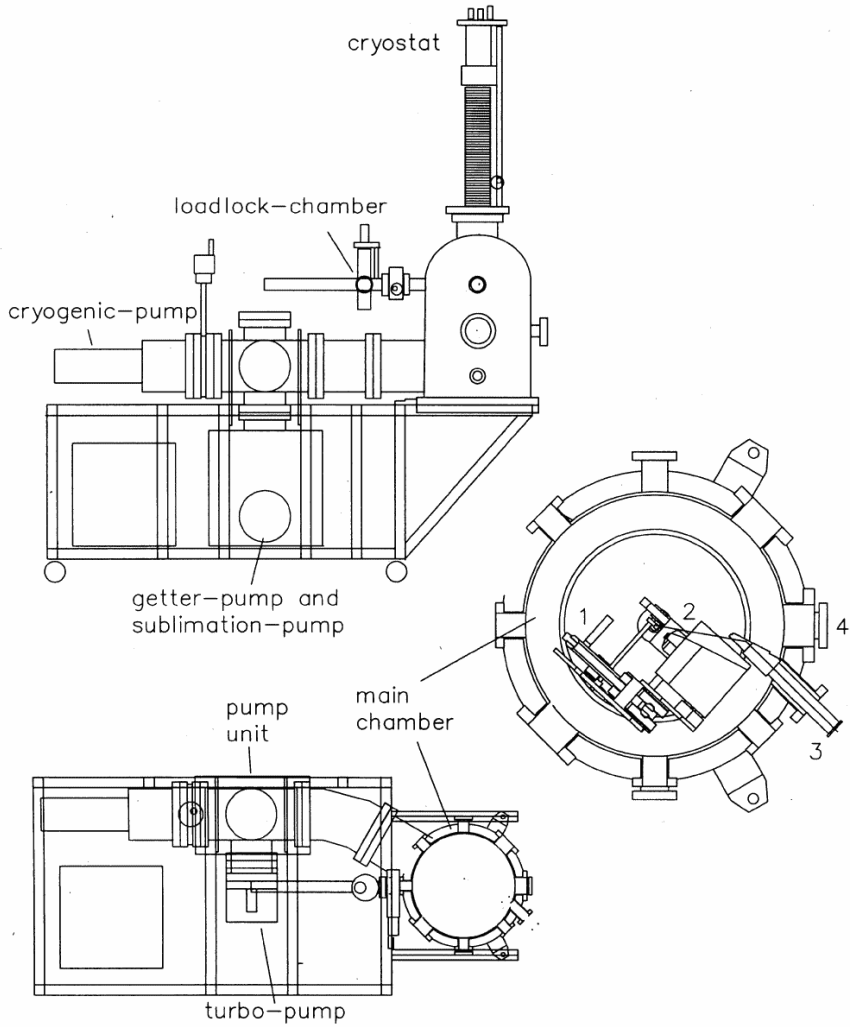


Photo Electron Spectrosopy

- powerfull technique to determine bandstructure and electronic properties of solids
- detected electrons easy to analyse
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- UHV conditions inevitable

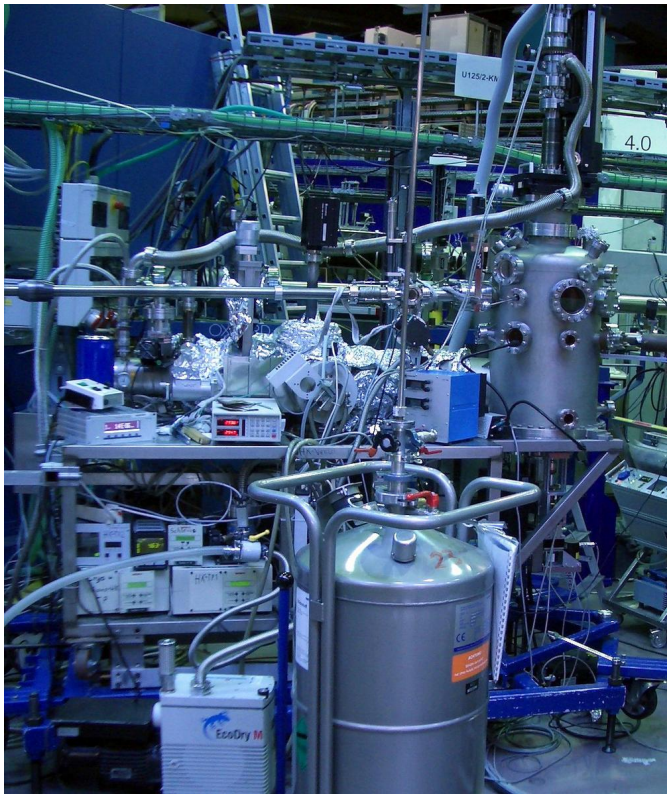
$Cd_xHg_{1-x}Te$

- first angle resolved measurement
- inverted bandstructure - zero gap
- complicated (110) surface preparation

Outlook

Measurement

- Laue pictures of measured crystals
- LEED at WESPHOA chamber
- EDX for composition
- automatic nitrogen refill system
- measurements at BESSY training beamline with syncrotron light and new Scienta
- cooled cleavage



More Samples ...

- samples of already grown $\mathrm{Cd_xHg_{1-X}Te}$ crystals from Hr. Sölle
- growth of new $\mathrm{Pb_xZn_{1-X}Te}$
- more samples from Moscow

Thanks for your attention!