

Определение Электронной Зонной Структуры $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ Методом Угловой Фотоэлектронной Спектроскопии

Семинар Кафедры Физики Низких Температур и Сверхпроводимости

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Arbeitsgruppe Elektronische Eigenschaften und Supraleitung

10. 12. 2007



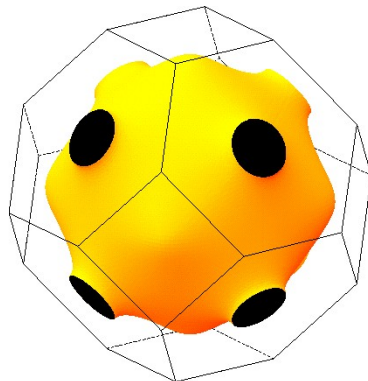
**МОСКОВСКИЙ
ГОСУДАРСТВЕННЫЙ
УНИВЕРСИТЕТ**
им. М.В.Ломоносова



Структура доклада

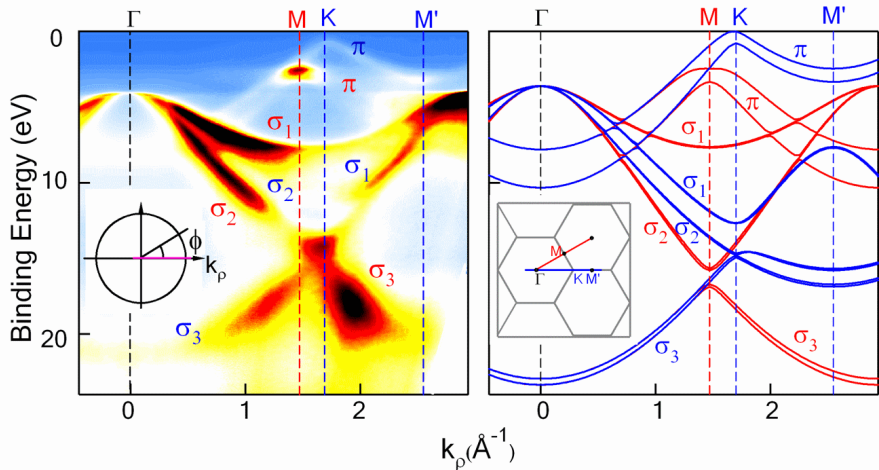
- 1 Мотивация
- 2 Угловая Фотоэлектронная Спектроскопия
 - Введение и базовые принципы
 - Энергетические соотношения и анализ
 - Устройство анализатора энергии
- 3 Качество поверхности, проверка и предсказания
 - Laue transmission pictures
 - Surface preparation by cleaving
 - Surface check by SEM, AFM and LEED
- 4 Результаты ARPES экспериментов на CdHgTe
 - Expected spectra and bandstructure
 - ARPES results and dispersion
 - Interpretation of results
- 5 Проблема, выводы и перспективы

The figure displays the energy band structure of GaAs. The vertical axis represents Energy in eV, ranging from -12 to 6. The horizontal axis represents the Wavevector k along high-symmetry directions: L, Λ , Γ , Δ , X, K, Σ , and Γ . The conduction bands are located above approximately 1.5 eV, with the Γ_6 band being the lowest. The valence bands are located below approximately -1.5 eV, with the Γ_8 band being the highest. The band structure shows characteristic features of a direct bandgap semiconductor, with the conduction band minimum and valence band maximum both occurring at the Γ point. The label 'GaAs' is placed in the upper right region of the plot.

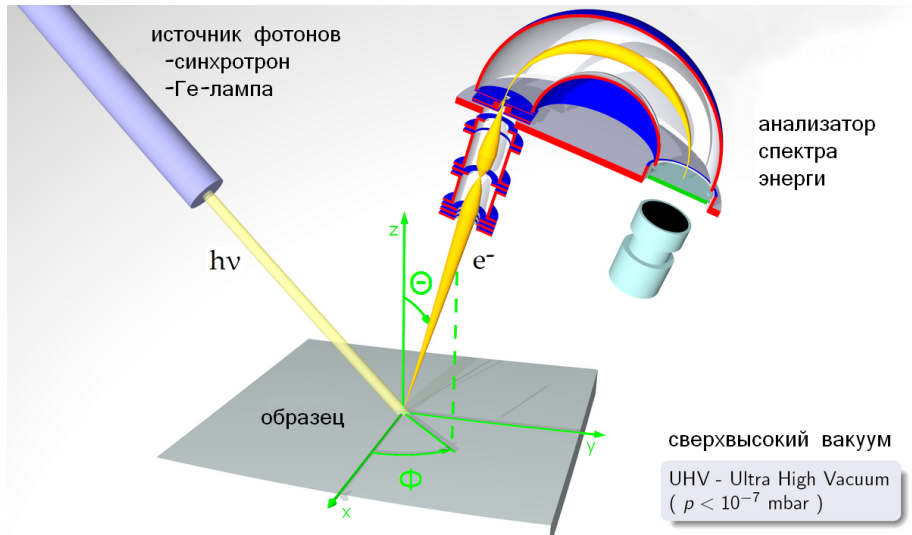


Экспериментальные результаты и теория

Спектроскопия фотоэлектронов на графите



Устройство ARPES



Первый шаг: Фотовозбуждение электрона

Вероятность перехода

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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Гамильтониан

The interaction between electron and photon is described by the Hamiltonian H_{WW} . In Coulomb gauge and linear approximation it is

$$H_{WW} = \frac{e}{2mc} \vec{A} \cdot \vec{p}$$

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Сохранение энергии

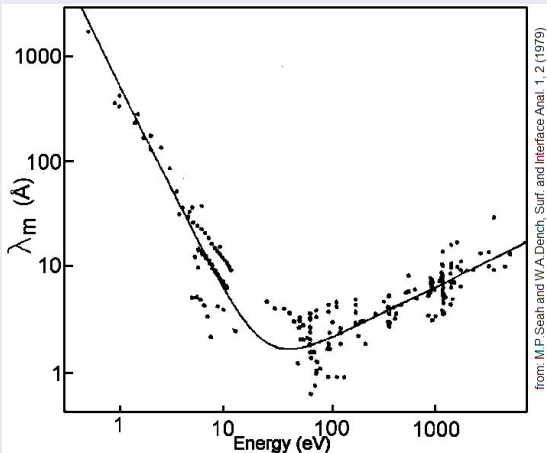
$$E_f = E_i + \hbar\omega$$

Сохранение импульса

$$\vec{k}_i = \vec{k}_f$$

Второй шаг: Транспорт фотоэлектронов к поверхности

Средний свободный пробег электронов в твёрдом веществе в зависимости от энергии



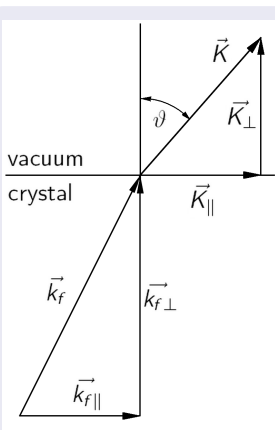
Ограничения метода

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.

Вторичные электроны

By scattering a spectra of low energy secondary electrons generates.

Третий шаг: Проникновение через поверхность



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

Дисперсия свободных электронов

Excited bulk state interacts with free electron state:

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

Отражение электронов на поверхности

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

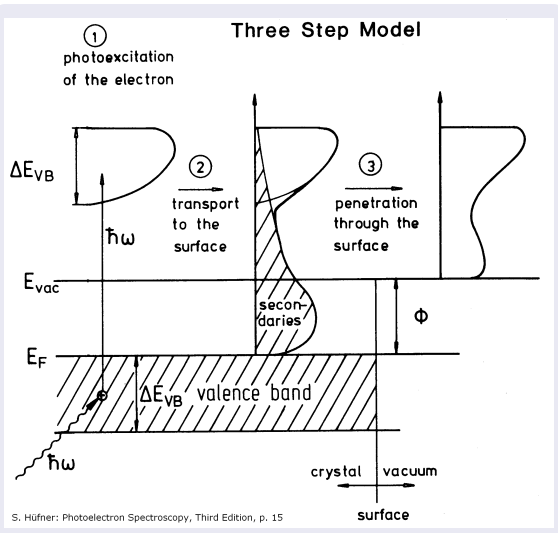
$$\vec{k}_{i||} = \vec{k}_{f||} = \vec{K}_{||} = \sqrt{\frac{2m}{\hbar}} E_{kin} \sin \vartheta$$

Final state energy and perpendicular component:

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

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

Энергетические соотношения во время измерения



Кинетическая энергия

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

Сила Лоренца

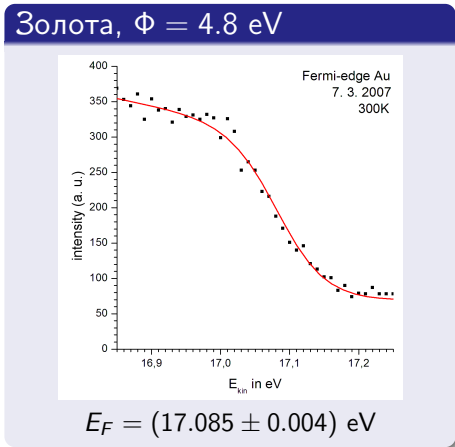
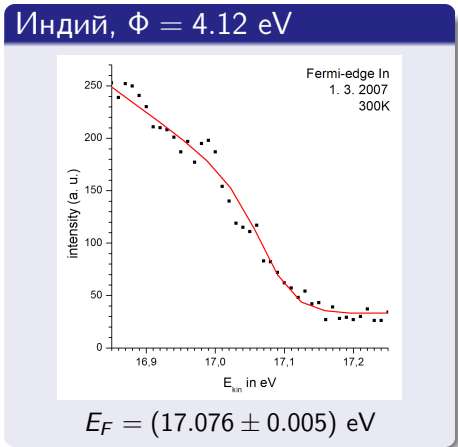
$$\vec{F} = q(\vec{E} + \vec{v} \times \vec{B})$$

$$B \leq 0.25 \mu T$$

Пример

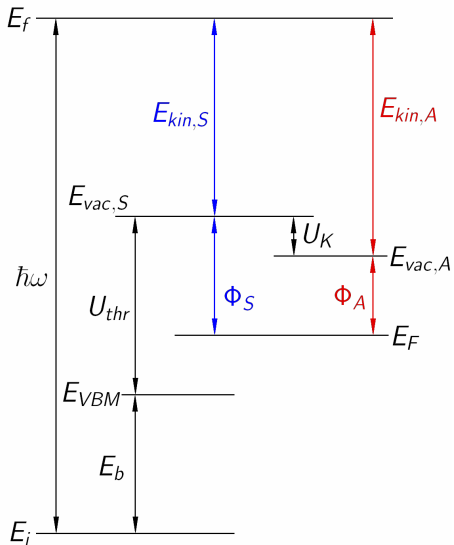
$\hbar\omega$	=	21.2eV	He-I
Φ	=	4.8eV	Au
E_{kin}	=	16.4eV	E_F

Зависит ли измеренная энергия E_F от работа выхода?



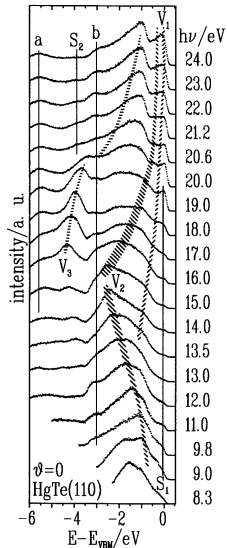
Измеренная величина энергии Ферми не зависит от работы выхода материала образца. Целая спектра сместилась во время измерения.

Работа выхода и отношения энергий

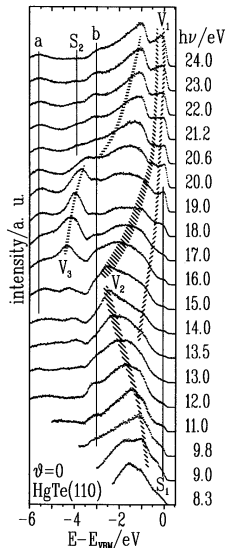
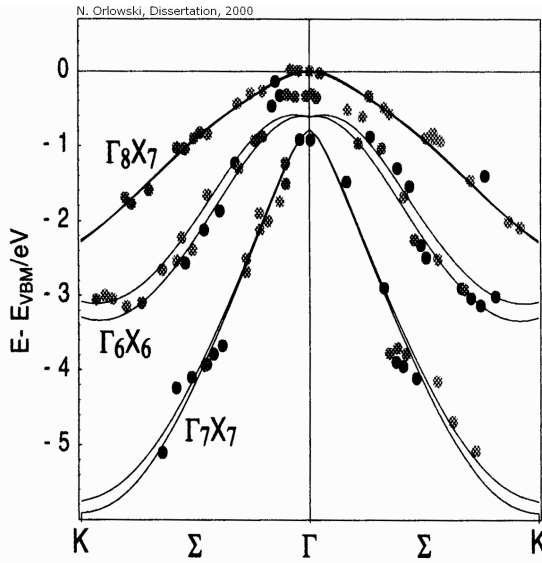


E_i	energy of initial state
E_F	energy of final state
E_{VBM}	valence band maximum
$E_{vac,S}$	vacuum level of sample
$E_{vac,A}$	vacuum level of analyser
$\hbar\omega$	photon energy
U_b	binding energy
E_{thr}	threshold of photo emission
$E_{kin,S}$	kinetic energy of electrons at the sample
$E_{kin,A}$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

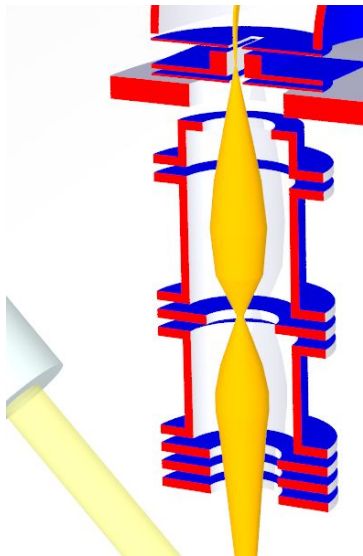
Fitting and resulting Band Structure



Fitting and resulting Band Structure



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

$$E_{kin,S} = 0.2 \text{ eV}$$

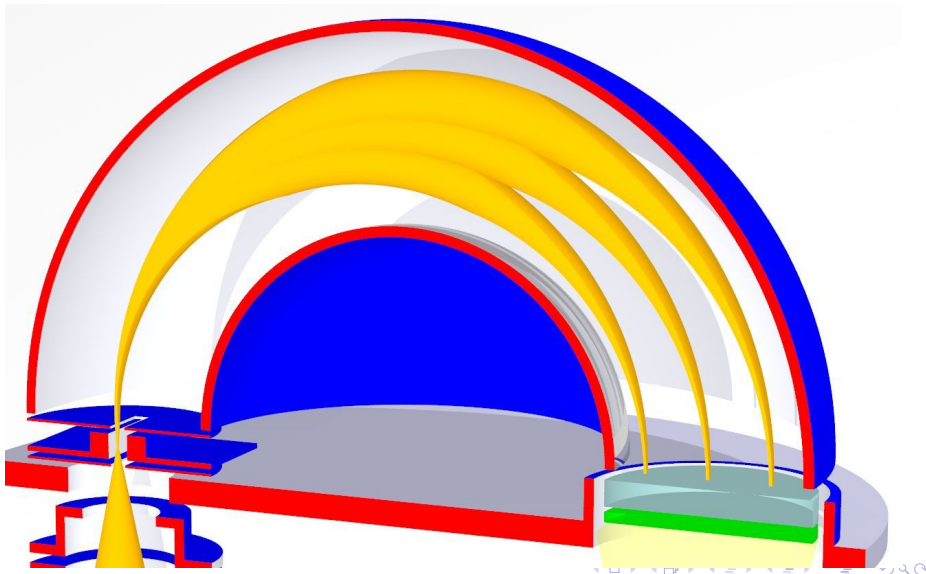
$$U_{ret} = 10.2 \text{ eV}$$

$$U_K = -0.4 \text{ eV}$$

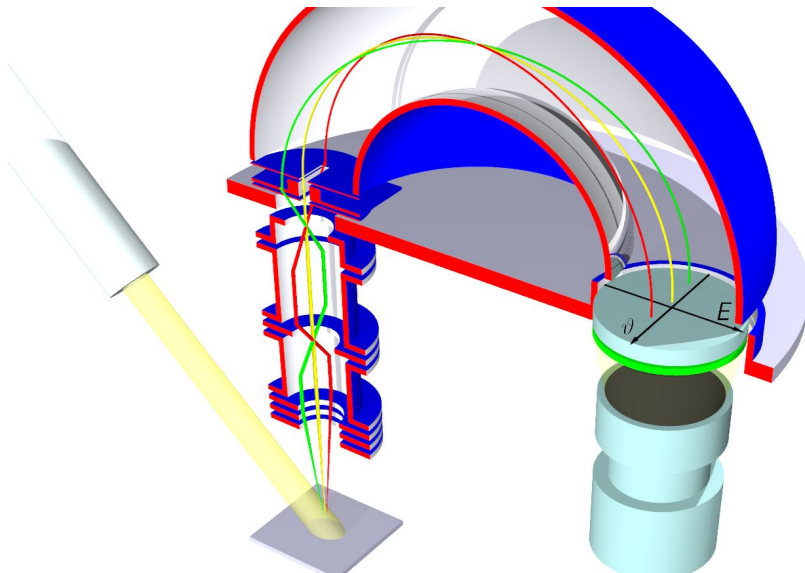
$$E_{pass} = 10 \text{ eV}$$

$$E_{kin,A} = -0.2 \text{ eV}$$

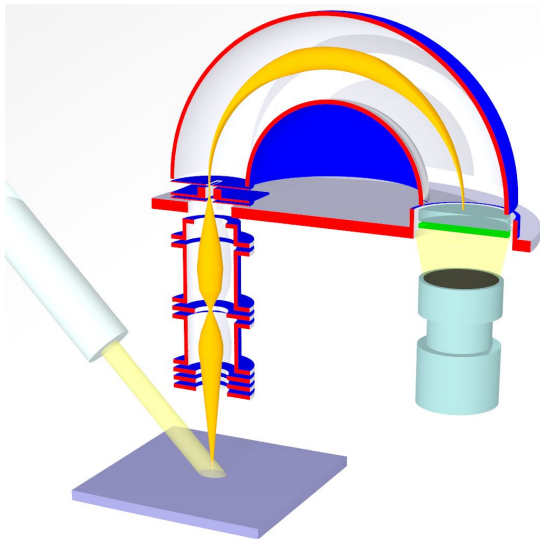
Energy Dispersion inside Spherical Condensator



Angle Resolution by Mapping of Entrance Point



Разрешение сферического анализатора



Potentials on hemispheres

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

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

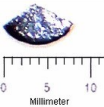
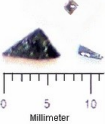
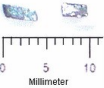
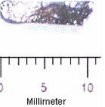
$$V_{in} = E_0[3 - 2(R_0/R_{in})]$$

Resolution

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

w width entrance slit
 α acceptance angle

Образцы $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$

№	I	II	III	IV	V	VI
						
value of X	0.07	0.4	0.2	0.183	0.1955	0.105
weight	186.3 mg	130.3 mg	158.5 mg	129.2 mg	248.5 mg	108.9 mg
orientation	<111>		<110>	<110>	<110>	<110>

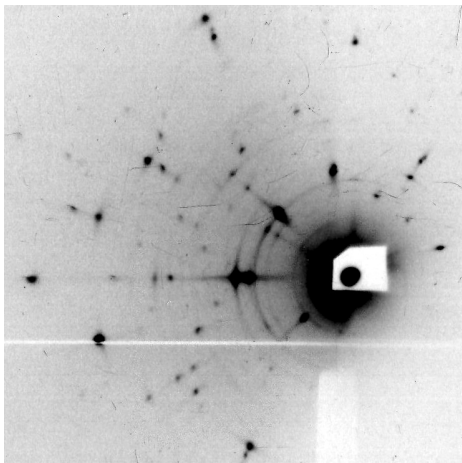
Образцы I по III

Frist the diploma thesis was based on these 3 samples. This work was announced for at least 2 years.

Образцы IV по VI

Further Samples Lennard Dudy brought from Moscow. Samples during measurement destroyed.

Проверка качества кристаллов методом Лауэ



Fringe rings

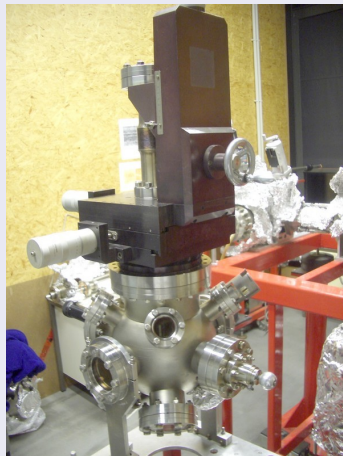
In this Laue transmission picture we see some rings that are typical for the Debye-Scherrer powder method. Accordingly this shows that our sample IV is not of perfect crystal quality. Rather there are some polycrystalline parts included in the sample. By the brightness of the other spots its amount can be assumed to be lower than 10 %

Surface Preparation - Cleavage Mechanism 1



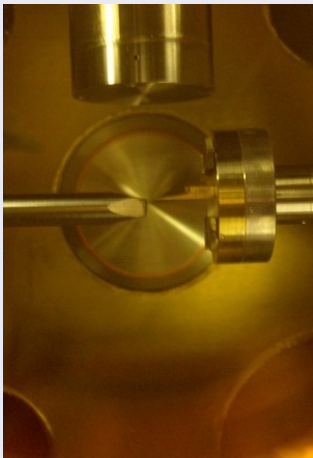
Spaltmechanismus, Norbert Orlowski, Doktorarbeit 2000

Norbert Orlowski 2000

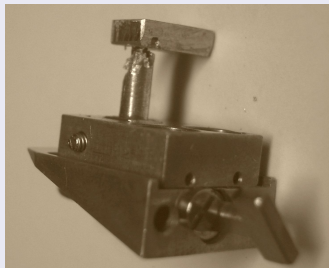
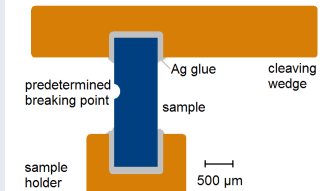


Matthias Kreier 2006

Surface Preparation - Cleavage Mechanism 2



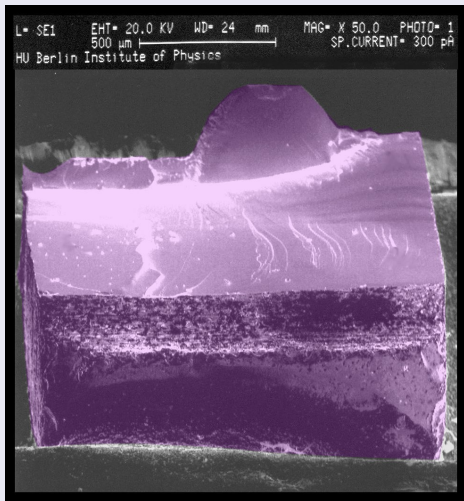
inside the cleavage chamber



cleavage in sample holder

First Surface Quality Check by SEM

SEM Image



SEM results

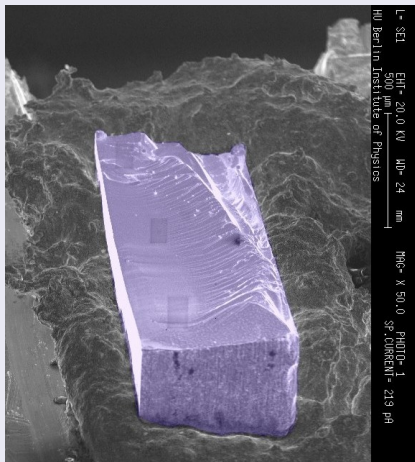
In front we see the predetermined breaking point - a sawn valley of 100 μm depth and the resulting cleavage. Already in this magnification a steplike surface structure can be observed. No flat surface as Van-der-Waals crystals show after cleavage.

Improvement

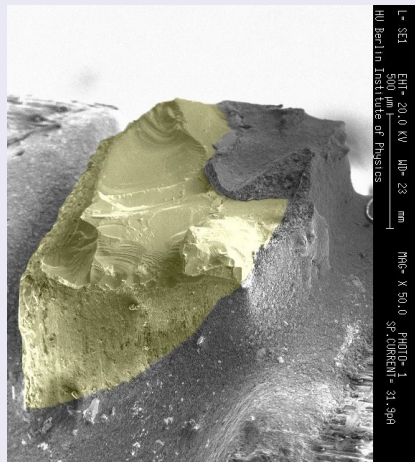
By cooled cleavage the surface quality improved tremendously. We used liquid Nitrogen to cool the samples down to 80 K and performed the cleavage.

Recent SEM pictures

Успешный раскол



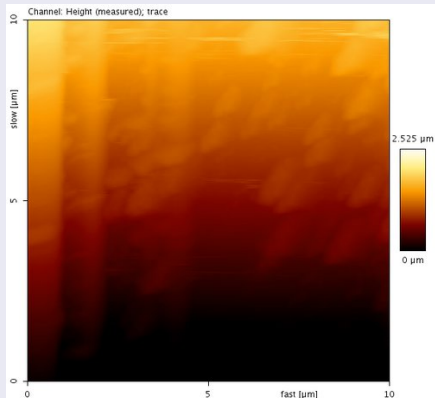
Неуспешный раскол



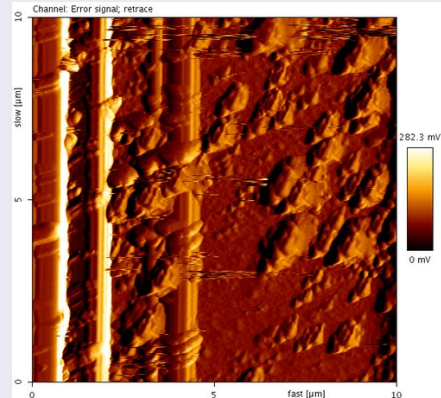
Исследование поверхности с AFM

AFM - Atomic Force Microscope (АСМ Атомный Силовой Микроскоп)

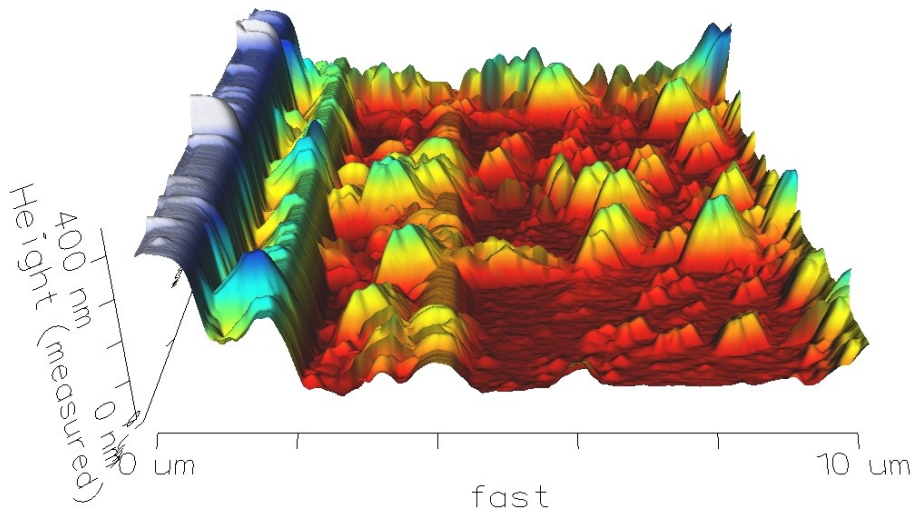
height measurement



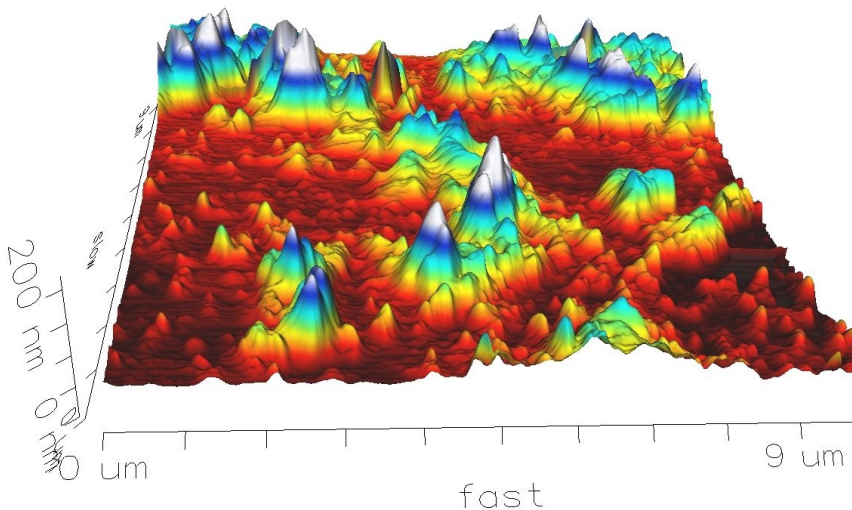
lateral deflection



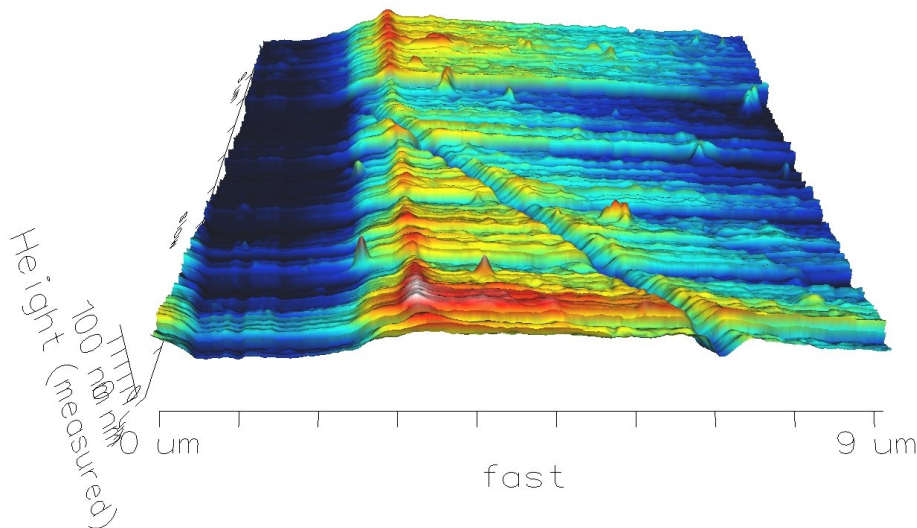
3D-Исследование поверхности, AFM



3D-Исследование поверхности образец № 3

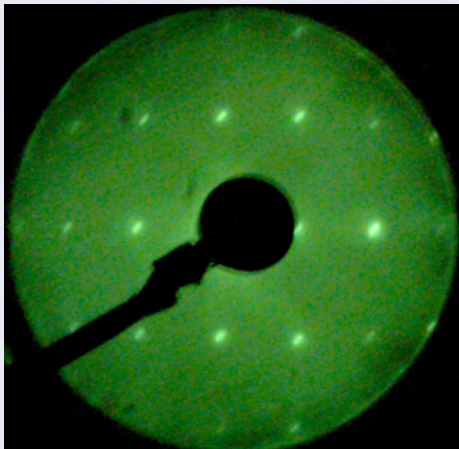


3D-Исследование поверхности образец № 5



Обследование качества поверхности LEED

LEED image at 156 eV



LEED method

The LEED method is very sensitive to overstructures - but we see a clean surface with constant periodicity. By the Laue formulae and the de Broglie relation

$$\vec{a}_1(\vec{k} - \vec{k}_0) = 2\pi h$$

$$\vec{a}_2(\vec{k} - \vec{k}_0) = 2\pi k$$

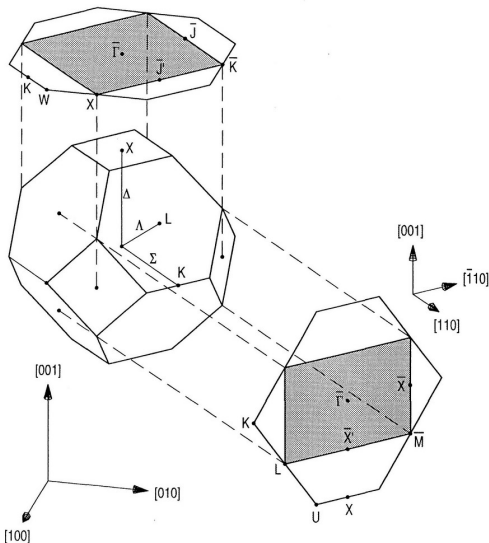
$$\lambda_{deBroglie} = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$$

with given Electron energy we get the lattice constants

$$a = 3.5 \text{ \AA} \quad b = 2.4 \text{ \AA}$$

of the observed sample.

Brillouin Zone of ZnS Crystals

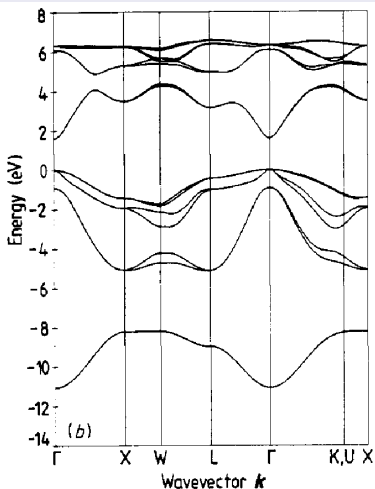


Dispersion perpendicular

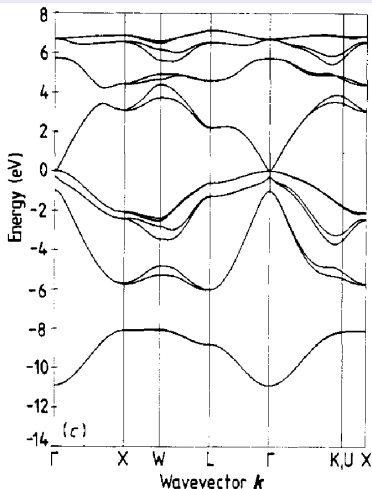
Volumen-Brillouin-Zone des fcc-Gitters mit hochsymmetrischen Punkten sowie die Oberflächen-Brillouin-Zonen der idealen (001) und (110)-Oberfläche. Die hochsymmetrischen Richtungen Delta, Sigma und Lambda, die den Richtungen [001], [110] und [110] entsprechen, sind ebenfalls eingezeichnet.

Ожидаемая структура зоны

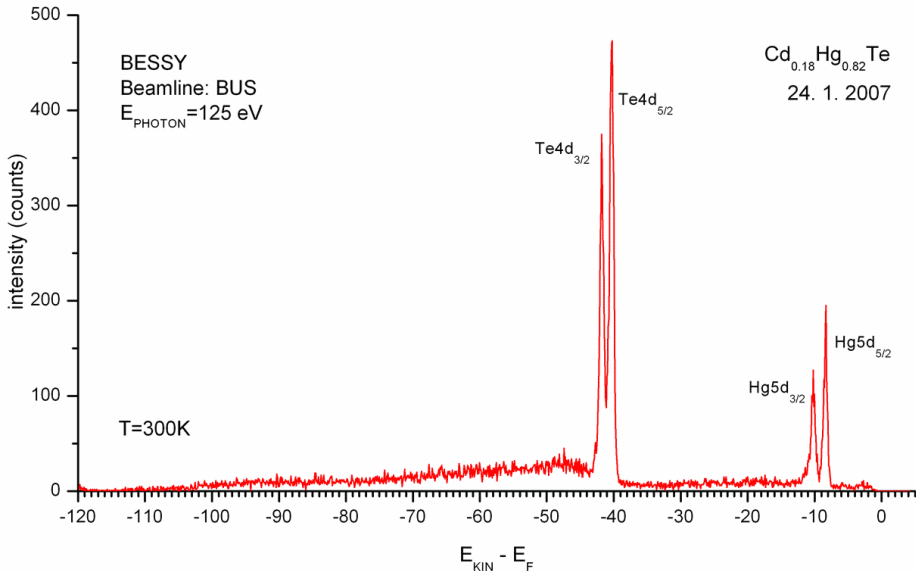
CdTe



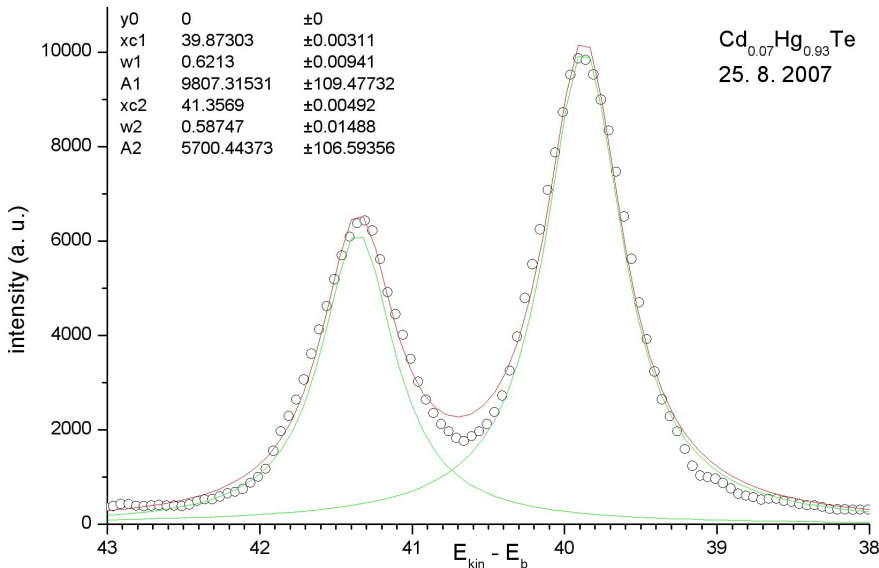
HgTe



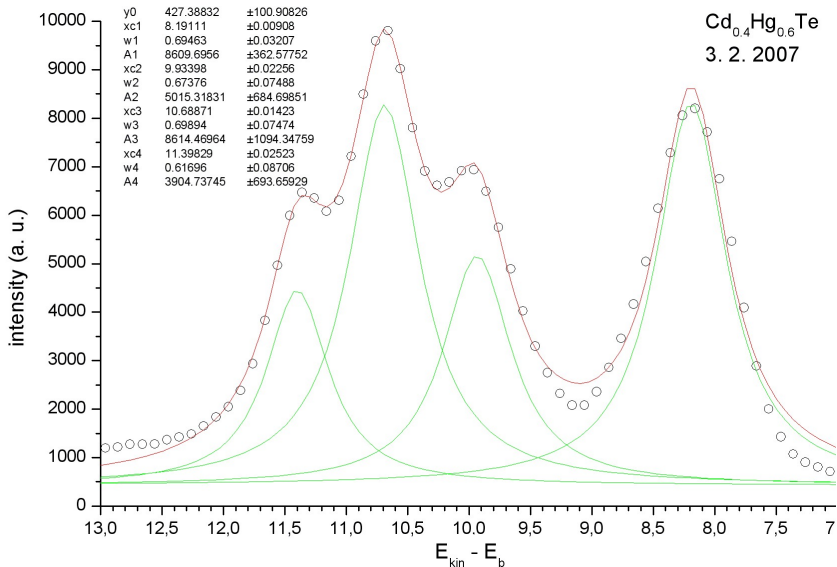
Результаты ARPES на BESSY, $\hbar\omega = 125$ eV



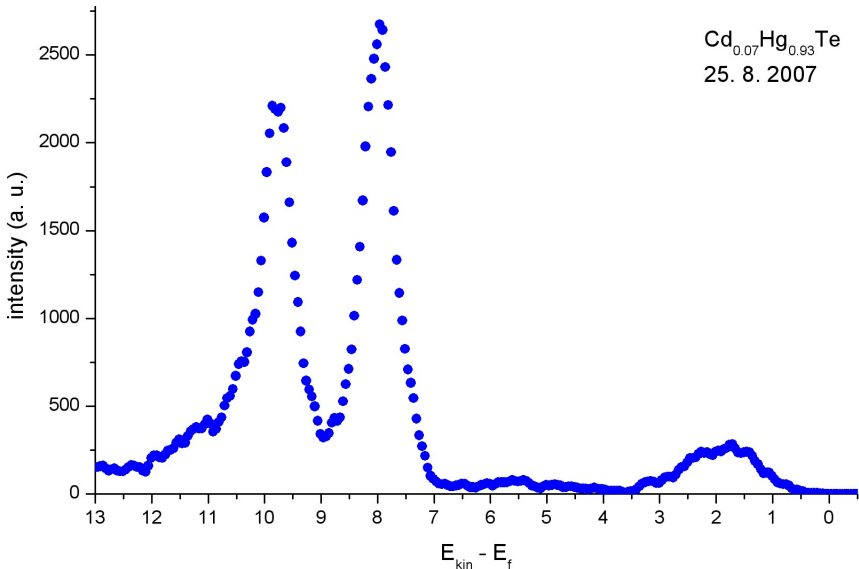
Core levels of $\text{Te}_{5/2}$ and $\text{Te}_{3/2}$



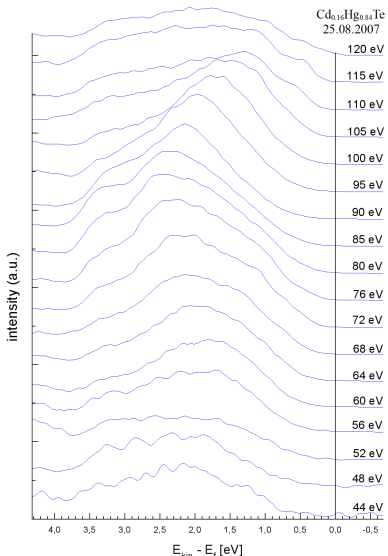
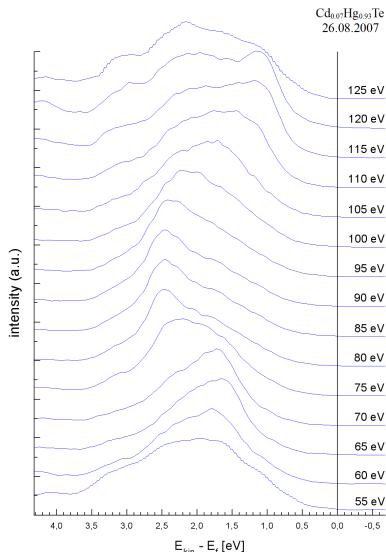
Core levels of $\text{Cd}_{5/2}$, $\text{Cd}_{3/2}$, $\text{Hg}_{5/2}$ and $\text{Hg}_{3/2}$



Valence band and core levels of Hg and Cd

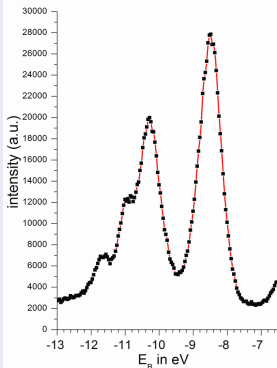


K-перпендикуляр: Дисперсия на CdHgTe



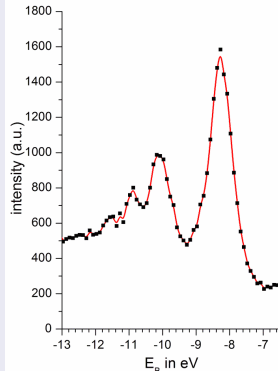
Core level shift depending on composition

BESSY $h\nu = 40$ eV



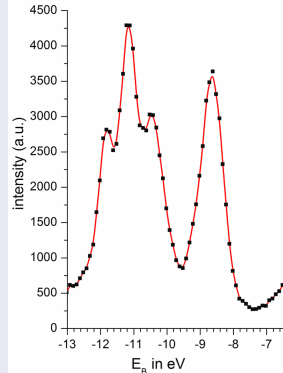
$\text{Cd}_{0.18}\text{Hg}_{0.82}\text{Te}$
26. 1. 2007

He-I $h\nu = 21.2$ eV



$\text{Cd}_{0.2}\text{Hg}_{0.8}\text{Te}$
8. 3. 2007

BESSY $h\nu = 80$ eV

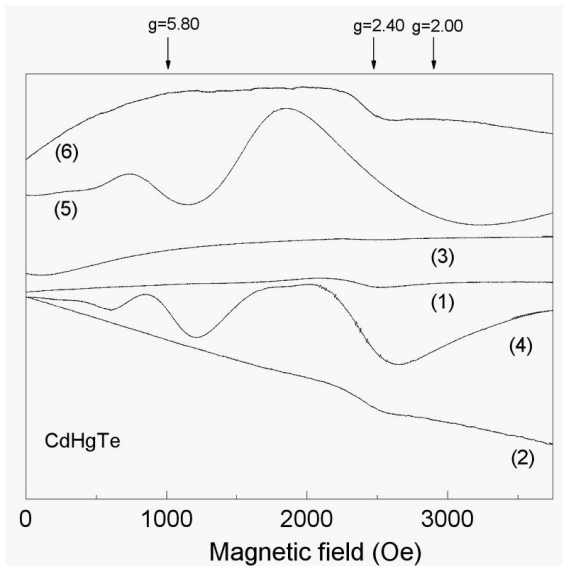


$\text{Cd}_{0.4}\text{Hg}_{0.6}\text{Te}$
3. 2. 2007

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)



Результаты EPR в Москве



Выводы

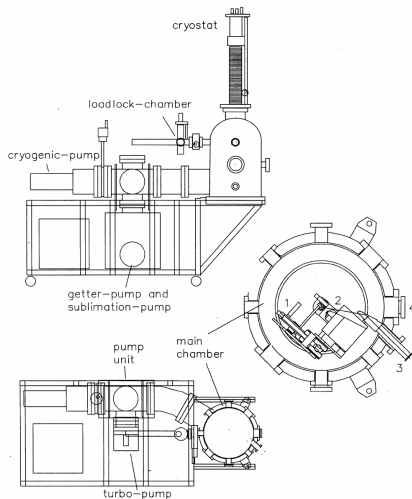


Photo Electron Spectroscopy

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

Выводы

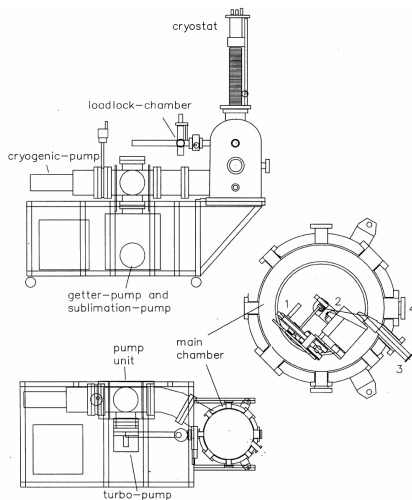


Photo Electron Spectroscopy

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

$\text{Cd}_x\text{Hg}_{1-x}\text{Te}$

- complicated surface preparation
- successful cooled cleavage
- bulk crystallinity is to question
- dispersion in angle resolved measurements

Перспективы

Исследования в Москве

- Determination of electron and hole mass
- Completed dispersion analysis
- Heat capacity measurement
- EPR on samples, SQUID

Обратно в Берлине

- Hall measurement of the samples in our workgroup by Dr. Dwelk
- Measurements at BESSY training beamline with synchrotron light and new Scienta
- Surface preparation by sputtering and annealing



Спасибо за внимание!

подробную информацию смотрите на

<http://people.physik.hu-berlin.de/~kreier/>