

FYS3410 - Vår 2010 (Kondenserte fasers fysikk)

<http://www.uio.no/studier/emner/matnat/fys/FYS3410/index-eng.xml>

Based on Introduction to Solid State Physics by Kittel

Course content

- Periodic structures, understanding of diffraction experiment and reciprocal lattice
- Imperfections in crystals: diffusion, point defects, dislocations
- Crystal vibrations: phonon heat capacity and thermal conductivity
- Free electron Fermi gas: density of states, Fermi level, and electrical conductivity
- Electrons in periodic potential: energy bands theory classification of metals, semiconductors and insulators
- Semiconductors: band gap, effective masses, charge carrier distributions, doping, pn-junctions
- Metals: Fermi surfaces, temperature dependence of electrical conductivity

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FYS3410 lecture schedule and exams: Spring 2010

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|--------------|---|----|
| M/18/1/2010: | Introduction and motivation. Periodicity and lattices | 2h |
| W/20/1/2010: | Index system for crystal planes. Crystal structures | 1h |
| M/25/1/2010: | Reciprocal space, Laue condition and Ewald construction | 2h |
| W/27/1/2010: | Brillouin Zones. Interpretation of a diffraction experiment | 1h |
| M/01/2/2010: | Crystal binding and introduction to elastic strain | 2h |
| W/03/2/2010: | Point defects, case study – vacancies | 1h |
| M/08/2/2010: | Point defects and atomic diffusion | 2h |
| W/10/2/2010: | Diffusion (continuation); dislocations | 1h |
| M/15/2/2010: | Crystal vibrations and phonons | 2h |
| W/17/2/2010: | Crystal vibrations and phonons | 1h |
| M/22/2/2010: | Planck distribution and density of states | 2h |
| W/24/2/2010: | Debye model | 1h |
| M/01/3/2010: | Einstein model and general result for density of states | 2h |
| W/03/3/2010: | Thermal conductivity | 1h |
| M/08/3/2010: | Free electron Fermi gas in 1D and 3D – ground state | 2h |
| W/10/3/2010: | Density of states, effect of temperature – FD distribution | 1h |
| M/15/3/2010: | Heat capacity of FEFG | 2h |
| W/17/3/2010: | Repetition | 1h |
| 22/3/2010: | Mid-term exam | |

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|---------------------|--|-----------|
| M/14/4/2010: | Electrical and thermal conductivity in metals | 2h |
| W/12/4/2010: | Bragg reflection of electron waves at the boundary of BZ | 1h |
| M/19/4/2010: | Energy bands, Kronig - Penny model | 2h |
| W/21/4/2010: | Empty lattice approximation; number of orbitals in a band | 1h |
| M/26/4/2010: | Semiconductors, effective mass method, intrinsic carriers | 2h |
| W/28/4/2010: | Impurity states in semiconductors and carrier statistics | 1h |
| M/03/5/2010: | p-n junctions and heterojunctions | 2h |
| W/05/5/2010: | surface structure, surface states, Schottky contacts | 2h |
| M/10/5/2010: | no lectures | |
| W/12/5/2010: | no lectures | |
| W/19/5/2010: | Repetition | 2h |
| W26/5/2010: | Repetition | 2h |
| 28/5/2010: | Final Exam (sensor: Prof. Arne Nylandsted Larsen at the Århus University, Denmark, http://person.au.dk/en/anl@phys.au.dk) | |

**Lecture 4: Bragg plains and Brillouin zones.
Use of diffraction experiment in research**

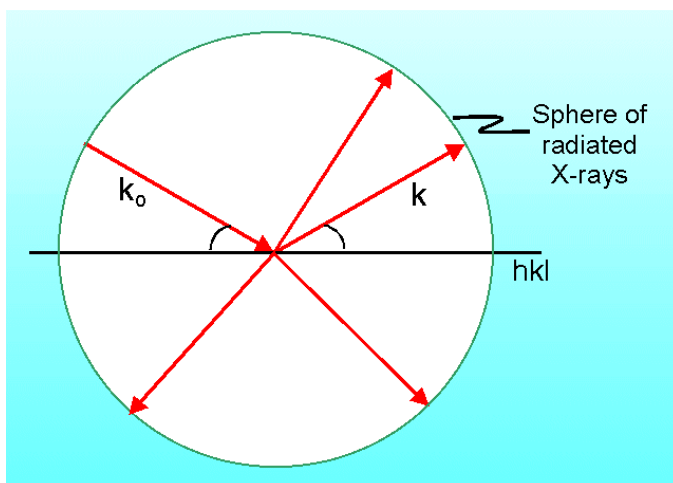
- repetition of Laue condition and Ewald construction;
- Introduction and interpretation of Brillouin zones;
- Use of diffraction experiment in research

Lecture 4: Bragg plains and Brillouin zones.
Use of diffraction experiment in research

- repetition of Ewald construction;
- Introduction and interpretation of Brillouin zones;
- Interpretation of x-ray diffraction measurements

Ewald construction

Laue assumed that each set of atoms could radiate the incident radiation in all directions

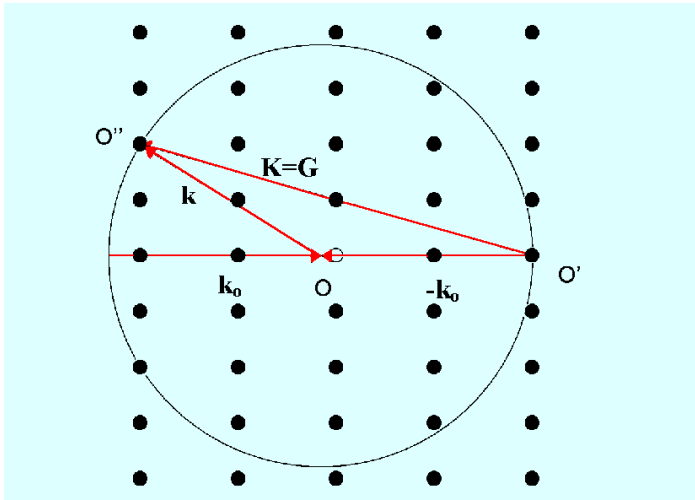


Constructive interference only occurs when the scattering vector, \mathbf{K} ($\Delta\mathbf{k}$ in the Kittel's notations), coincides with a reciprocal lattice vector, \mathbf{G}

This naturally leads to the Ewald Sphere construction

Ewald construction

We superimpose the imaginary “sphere” of radiated radiation upon the reciprocal lattice



Draw sphere of radius $1/\lambda$ centred on end of \mathbf{k}_0

Reflection is only observed if sphere intersects a point

i.e. where $\mathbf{K}=\mathbf{G}$

Lecture 4: Brillouin zones. Interpretation of a diffraction experiment

- repetition of Laue condition and Ewald construction;
- Introduction and interpretation of Brillouin zones;
- Interpretation of x-ray diffraction measurements

Bragg planes and Brillouin zone construction

The construction of Bragg Planes in the context of Brillouin zones can be understood by considering Bragg's Law $\lambda = 2d\sin\theta$. As we now know, in reciprocal space this can be expressed in the form

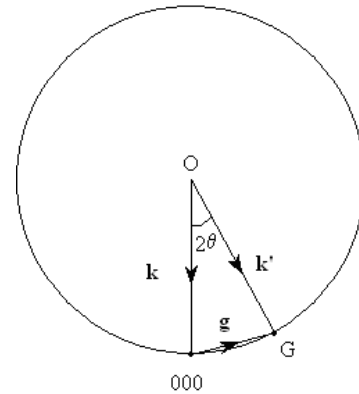
$$\mathbf{k}' - \mathbf{k} = \mathbf{g}$$

where \mathbf{k} is the wave vector of the incident wave of magnitude $2\pi/\lambda$,

\mathbf{k}' is the wave vector of the diffracted wave, also of magnitude $2\pi/\lambda$, and

\mathbf{g} is a reciprocal lattice vector of magnitude $2\pi/d$:

As we also know, this can be illustrated graphically using the Ewald sphere construction – with 000 to be the origin of the reciprocal lattice and O is the centre of the sphere of radius $|\mathbf{k}|$.



Bragg planes and Brillouin zone construction

If the angle subtended at O between 000 and \mathbf{G} on the diagram is 2θ , simple geometry shows that

$$\sin \theta = \frac{|\mathbf{g}|}{2|\mathbf{k}|} = \frac{\frac{2\pi}{d_{\mathbf{hk}}}}{2 \cdot \frac{2\pi}{\lambda}} = \frac{\lambda}{2d_{\mathbf{hk}}} \quad \lambda = 2d_{\mathbf{hk}} \sin \theta$$

The equation

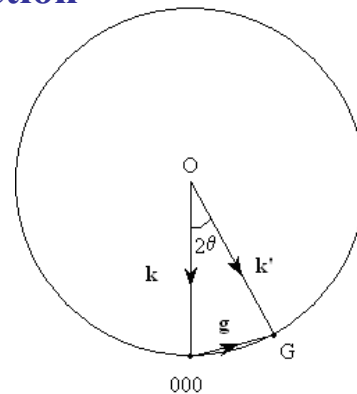
$$\mathbf{k}' - \mathbf{k} = \mathbf{g}$$

can be rearranged in the form

$$\mathbf{k}' = \mathbf{k} + \mathbf{g} \text{ so that}$$

$$\mathbf{k}' \cdot \mathbf{k}' = (\mathbf{k} + \mathbf{g}) \cdot (\mathbf{k} + \mathbf{g}) = \mathbf{k} \cdot \mathbf{k} + \mathbf{g} \cdot \mathbf{g} + 2\mathbf{k} \cdot \mathbf{g}$$

But $\mathbf{k}' \cdot \mathbf{k}' = \mathbf{k} \cdot \mathbf{k}$ because diffraction is an elastic scattering event,



$$\mathbf{g} \cdot \mathbf{g} + 2\mathbf{k} \cdot \mathbf{g} = 0$$

Bragg planes and Brillouin zone construction

$$\mathbf{g} \cdot \mathbf{k} + 2\mathbf{k} \cdot \mathbf{g} = 0$$

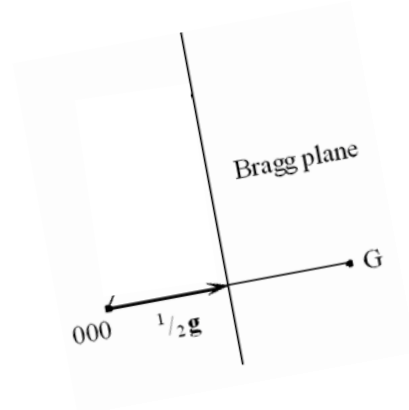
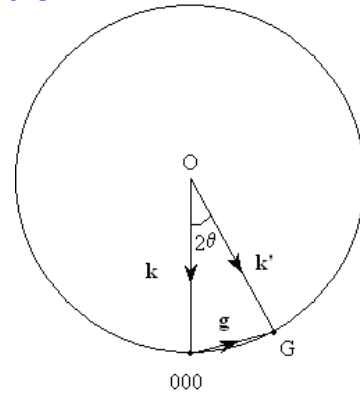
To construct the Bragg Plane, it is convenient to replace \mathbf{k} by $-\mathbf{k}$ in this equation so that both \mathbf{k} and \mathbf{g} begin at the origin, 000, of the reciprocal lattice. Hence, the equation can be written in the form

$$\mathbf{k} \cdot (\frac{1}{2}\mathbf{g}) = (\frac{1}{2}\mathbf{g}) \cdot (\frac{1}{2}\mathbf{g})$$

Constructing the plane normal to \mathbf{g} at the midpoint, $(\frac{1}{2}\mathbf{g})$,

then means that **any** vector \mathbf{k} drawn from the origin, 000, to a position on this plane satisfies the Bragg diffraction condition.

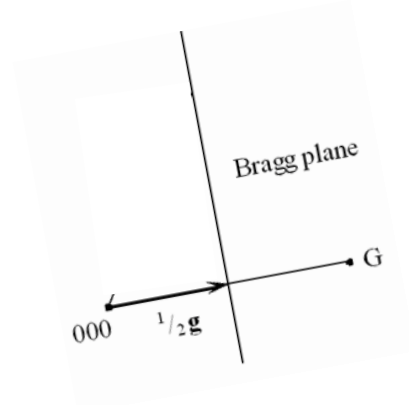
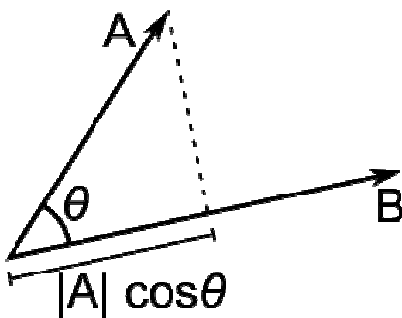
Do we understand this? Let's repeat



Bragg planes and Brillouin zone construction

$$\mathbf{k} \cdot (\frac{1}{2}\mathbf{g}) = (\frac{1}{2}\mathbf{g}) \cdot (\frac{1}{2}\mathbf{g}) \quad \text{When this holds – diffraction occurs – that's the law}$$

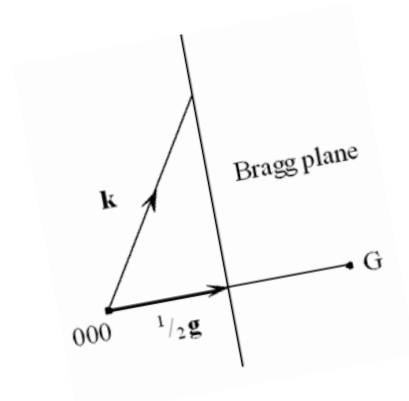
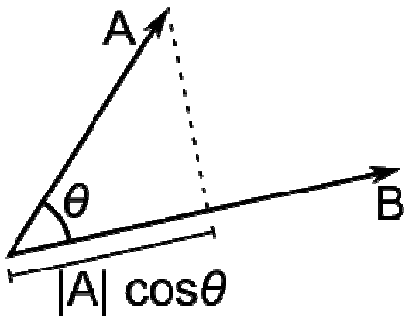
Let's consider when this "dot" products will do coincide?
What the dot product by the way?



Bragg planes and Brillouin zone construction

$\mathbf{k} \cdot (\frac{1}{2}\mathbf{g}) = (\frac{1}{2}\mathbf{g}) \cdot (\frac{1}{2}\mathbf{g})$ When this holds – diffraction occurs – that's the law

Let's consider when this "dot" product will coincide?
What the dot product by the way?

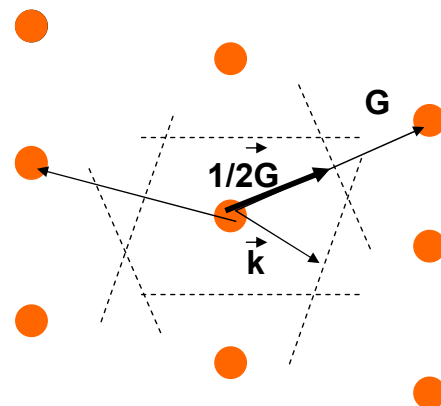


Fundamental conclusion is:

A wave with a wave vector $k < k_c$ has no chance to get diffracted

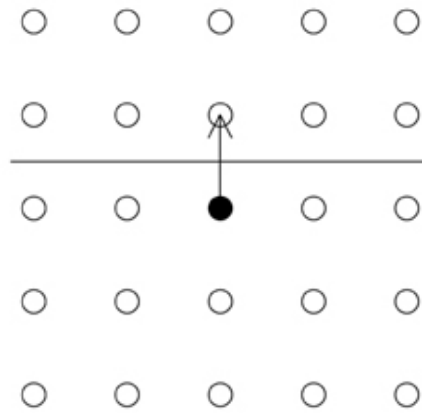
Bragg planes and Brillouin zone construction

The vector \mathbf{k}_{in} (also \mathbf{k}_{out}) lies along the perpendicular bisecting plane of a \mathbf{G} vector

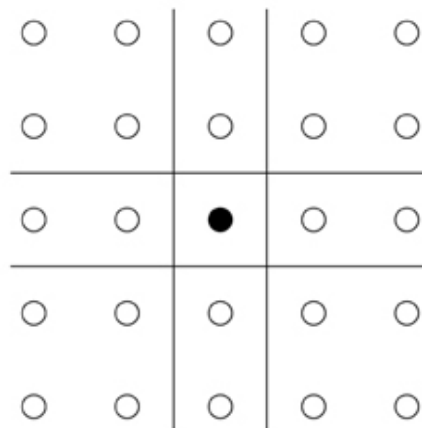


- Brillouin Zone formed by perpendicular bisectors of \mathbf{G} vectors
- Consequence: No diffraction for any \mathbf{k} inside the first Brillouin Zone
- Special role of Brillouin Zone (Wigner-Seitz cell of reciprocal lattice) as opposed to any other primitive cell

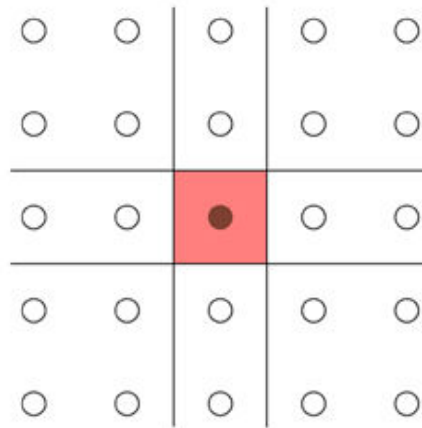
Bragg planes and Brillouin zone construction



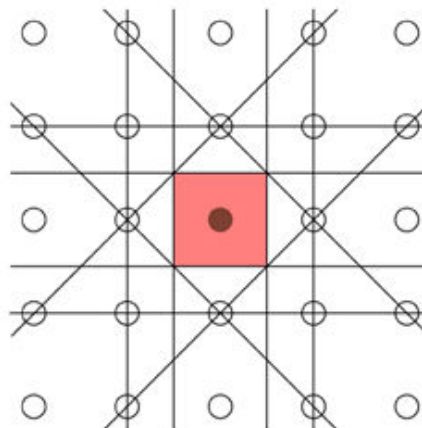
Bragg planes and Brillouin zone construction



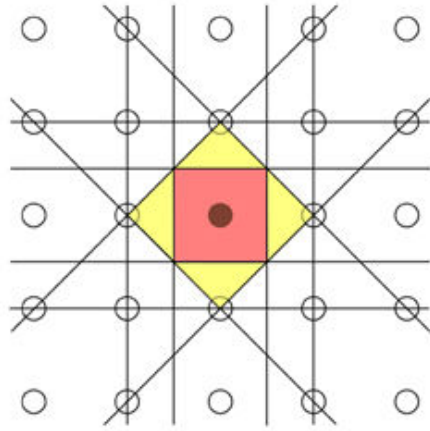
Bragg planes and Brillouin zone construction



Bragg planes and Brillouin zone construction



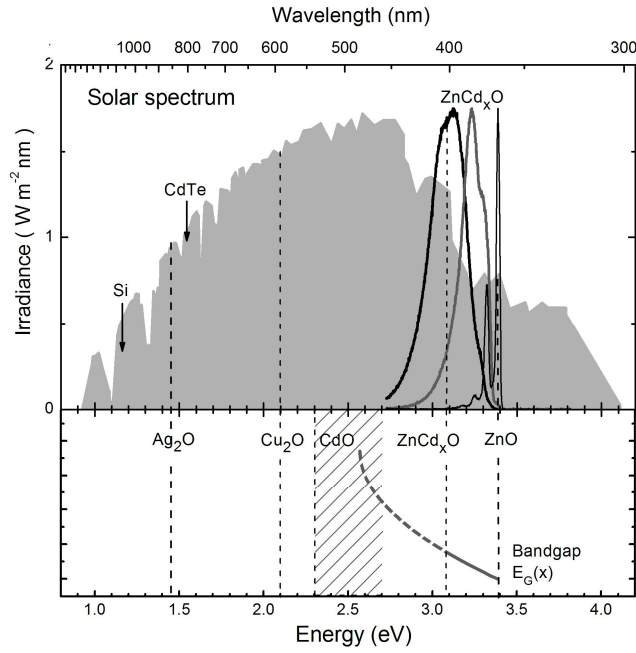
Bragg planes and Brillouin zone construction



Lecture 4: Bragg plains and Brillouin zones. Use of diffraction experiment in research

- repetition of Laue condition and Ewald construction;
- Introduction and interpretation of Brillouin zones;
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Use of diffraction experiment in research



Schematic of the structures studied

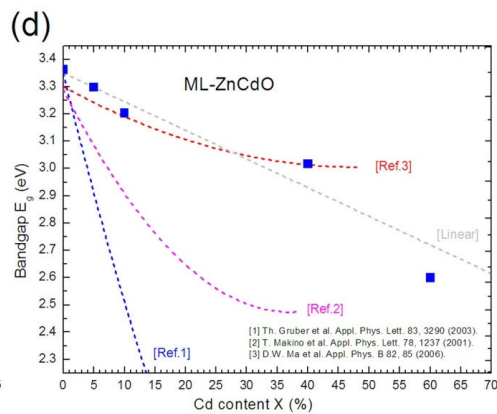
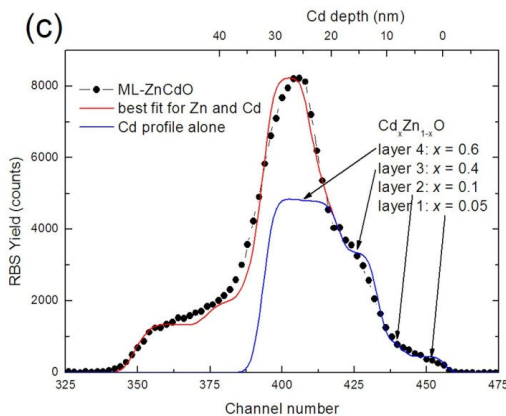
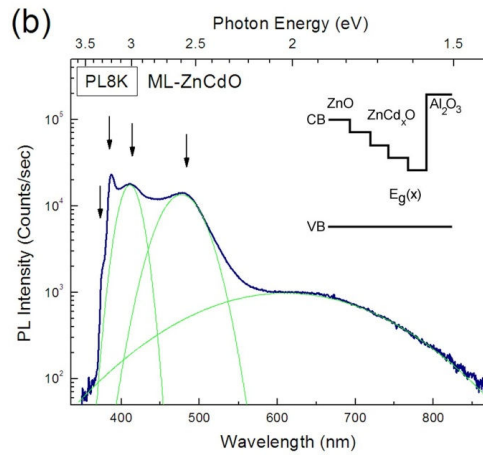
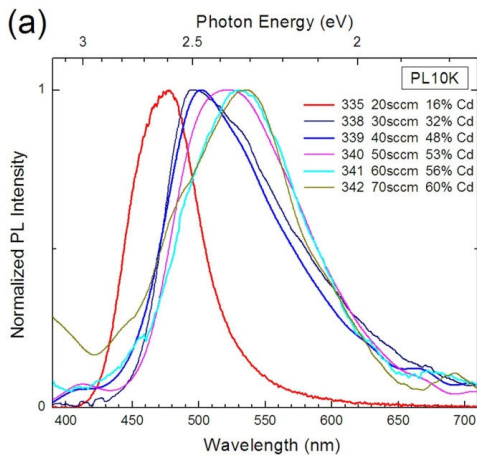
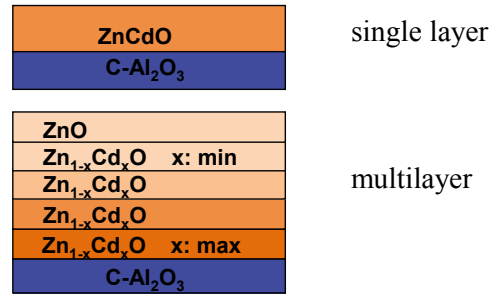
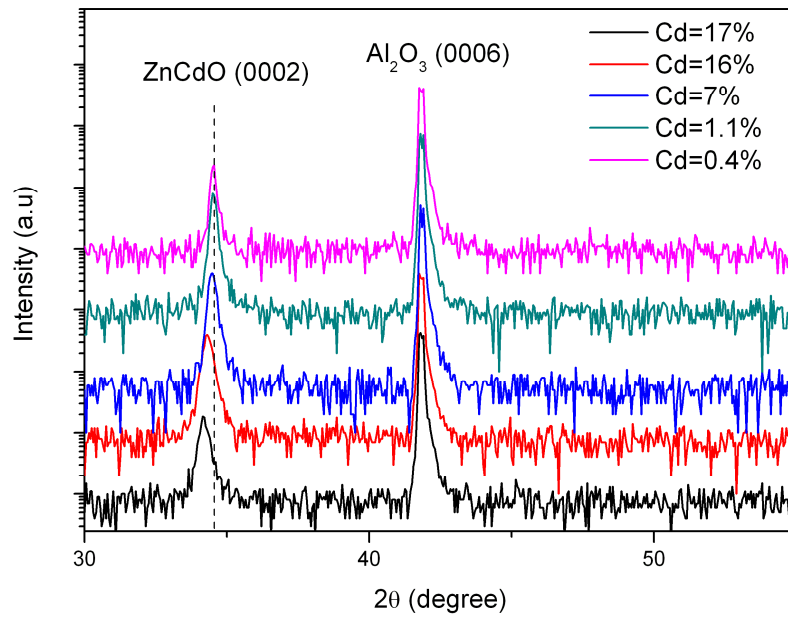


FIG. 1. (a) Typical photoluminescence (PL) spectra from ZnCdO films as a function of Cd content; (b) PL spectrum of a ML-structure as recorded at 8K with a schematics of the band gap in the inset; (c) Cd profile through ML-structure as measured by RBS; (d) our results in the context of literature.

Use of diffraction experiment in research



Use of diffraction experiment in research

