

*Nan* ••• **ED**

## NanED Workshop II

XRPD, Intellectual properties,  
Diffraction on imperfect crystals



Johannes Gutenberg University  
Mainz, December 6.-8.

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Hotel INNdependence

Electron Microscopy Centre  
Mainz

**EMC-M**

# Crystalline Material (micro or nano crystalline)

3DED

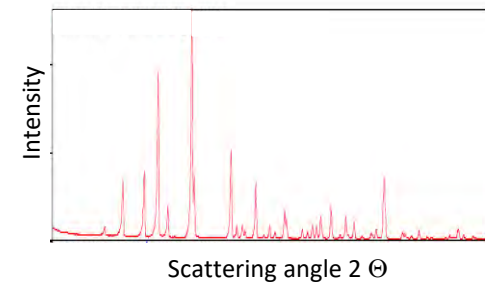
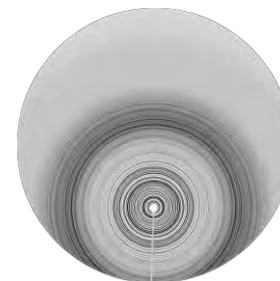
Diffraction on a single nano crystal



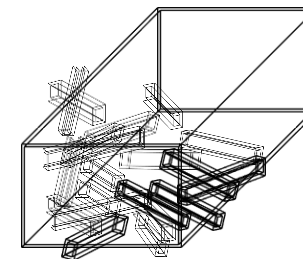
- Information from only one crystal
- Textured material: long axis intensities missing
- In situ experiments difficult

XRPD

Diffraction on thousands of crystals

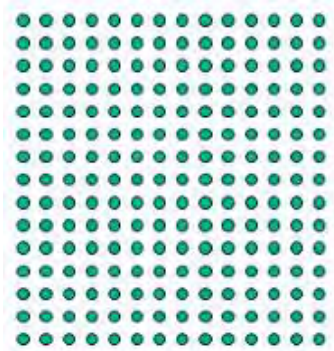


- Information from the whole sample
- Long axis intensities enhanced
- In situ experiments easier

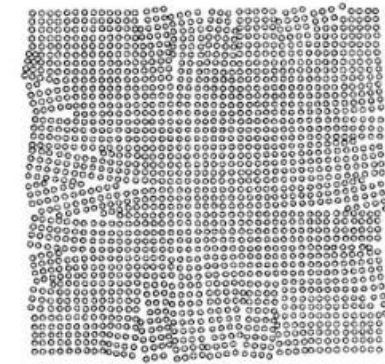


XRPD in pharmaceutical industry  
Intellectual properties and patents

# Imperfect crystals – disordered material

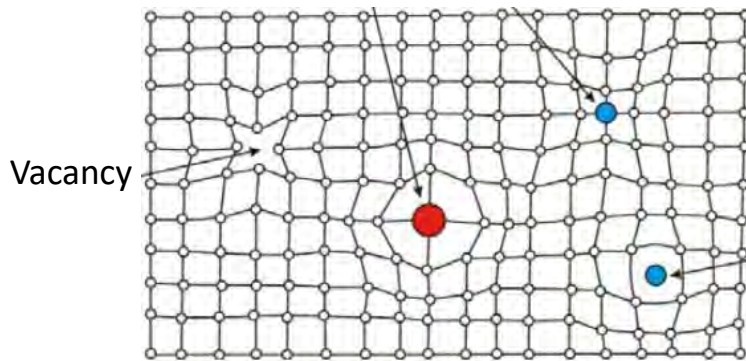


Any deviation from perfect periodicity in a crystal structure.



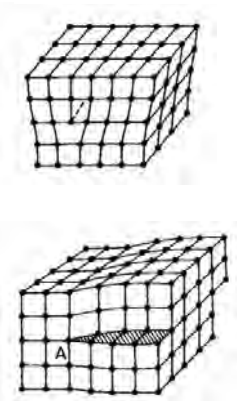
Substitution

Dislocations

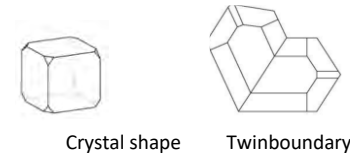


Vacancy

Interstitial atom

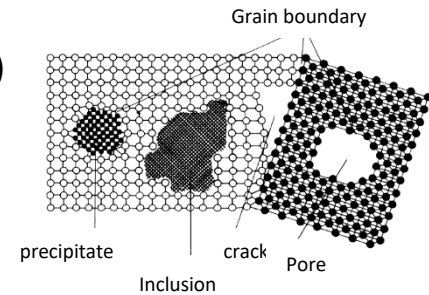


- Stacking faults
- Anti phase boundary
- Grain boundary (small angle)



Crystal shape

Twinboundary



precipitate

Inclusion

crack

Pore

Diss. Th. W. Loewenhoff, Bonn 2008

0D  
Point defect  
3D diffuse

1D  
Line defect  
2D diffuse

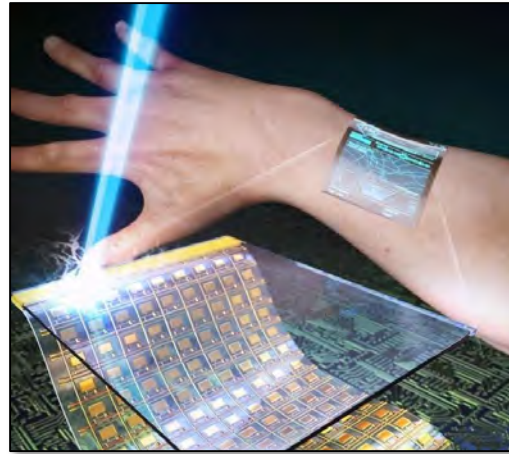
2D  
Planar defect  
1D diffuse

3D  
Volume defect  
0D diffuse



LEDs

rubapt.com



Thin film transistors

Ceramics.org



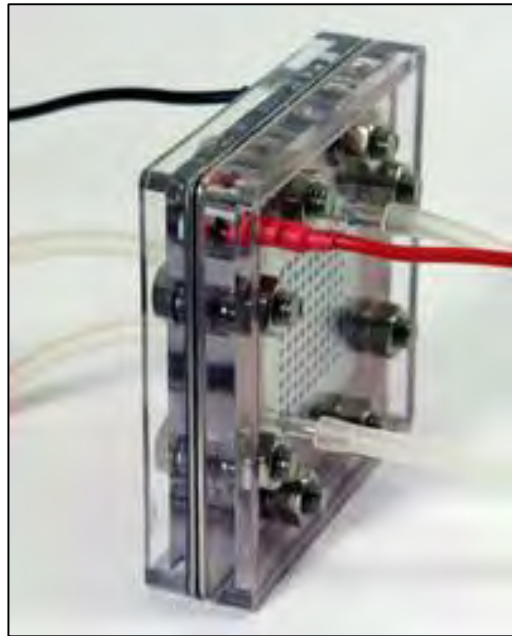
Solar cells

Wikipedia.org



Kemet.com

Piezo- and ferroelectrics  
(non-volatile memory)

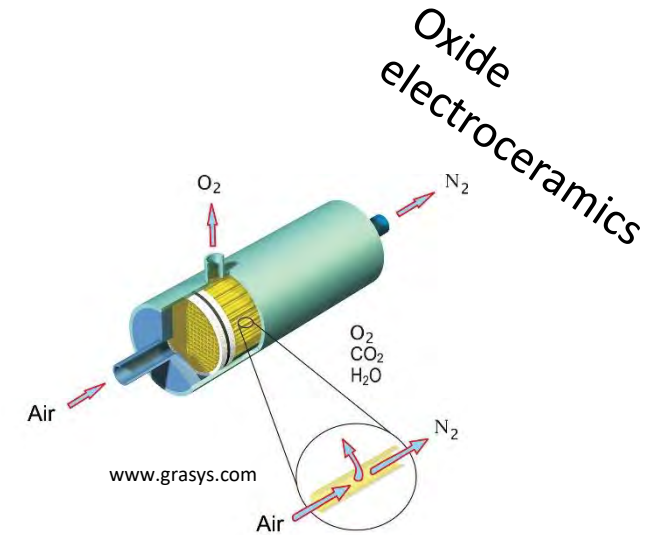


Planet-schule.de



www.daparto.at

Semiconducting oxides



## Tuesday December 6.12.

08:30 – 09:00 **Welcome and introduction:** Ute Kolb, University Mainz

09:00 – 09:30 **XRPD measurement techniques:** Nicolas Barrier, CNRS Caen

09:30 – 10:00 **XRPD on synchrotron sites:** Jasper Plaisier, Elettra Sincrotrone Trieste

*10:00 – 10:30 Coffee break*

10:30 – 11:15 **XRPD – structure solution and refinement strategies:** Robert Dinnebier, MPI Stuttgart

11:15 – 11:45 **Intellectual properties and patent in science:** Tina Einfeld, BASF, Ludwigshafen

*12:00 – 13:00 Lunch*

13:00 – 14:30 **Students presentations I (Projects # 1, 2, 4, 5, 7, 3\*, 10\* each 10min) \*Online**

14:30 – 18:00 Two parallel practical sessions (including a **coffee break**)

Session I: **Visit of the TEM facilities at the University, demo FAST-ADT and eADT (Tram Pariser Tor)**

Session II: **EXPO (Corrado Cuocci, Bari), X'Pert (Nicolas Barrier), TOPAS (Sebastian Bette)**

*Visit of Christmas Market (meet at 20:00 @ Eisgrubbräu, Weißliliegasse 1A)*



Tutorial @ Electron Microscopy Centre  
Mainz **EMC-M**

Travel by Tram 14:34

**Pariser Tor to Friedrich von Pfeiffer Weg**



Building 2121  
Duesbergweg 10-14



Campusbrücke



By foot

**Wednesday December 7.12.**

08:30 – 09:00 **XRPD – on pharmaceuticals:** Norbert Nagel, AbbVie, Ludwigshafen

09:00 – 09:30 **XRPD – Refinement of disordered inorganics:** Sebastian Bette, MPI Stuttgart

09:30 – 10:00 **XRPD – challenging organic disordered structures:** Martin U. Schmidt, University Frankfurt

**10:00 – 10:30 Coffee break**

10:30 – 11.15 **The nature of total scattering – theoretical aspects:** Jan Pieter Abrahams, PSI, Basel

11:15 – 11:45 **Precession and quasi-parallel electron diffraction-an electron optics perspective:** Sergi Plana Ruiz, University Rovira i Virgili, Tarragona

**12:00 – 13:00 Lunch**

**13:00 – 14:30 Students' presentations II (Project # 8, 9, 11, 12, 13, 15 each 10min)**

14:30 – 18:00 Two parallel practical sessions (including a **coffee break**)

Session I: **Visit of the TEM facilities at the University, demo FAST-ADT and eADT**

Session II: **EXPO (Corrado Cuocci, Bari), X'Pert (Nicolas Barrier), TOPAS (Sebastian Bette)**

**19:00 Dinner @ Bootshaus, Victor-Hugo-Ufer 1**



**Menu (according to your preliminary choice)**

<u>Aperitif:</u>	Homemade X-MAX punch, choice: alcoholic or non-alcoholic
<u>Finger food:</u>	Goat cheese praline with beetroot and Asian Teriyaki-Sesam-Chicken
<u>Appetizer:</u>	Lamb's lettuce   potato dressing   bacon   croutons
<u>Main course:</u>	Duck breast   thyme – orange juice   red cabbage   potato dumplings
<u>Veget. M. course:</u>	Pumpkin Risotto   goat cheese   caramelized walnuts
<u>Dessert:</u>	Curd mousse   winter spices   orange

**Thursday December 8.12.**

We start earlier this day !!!

08:00 – 08:45 **Pair distribution function PDF:** Reinhard Neder, University Erlangen

08:45 – 09:30 **Introduction to 3D-PDF:** Ella Schmidt, University Bremen

09:30 – 10:00 **Defect structures investigated with 3DED:** Ute Kolb, University Mainz

10:00 – 10:30 **Coffee break**

10:30 – 12:00 Session 1: **DISCUS Basics and 1D-PDF** (Reinhard Neder/Ella Schmidt)

12:00 – 13:00 **Lunch**

13:00– 15:00 Session 2: **eADT (Ute Kolb), DISCUS 3D-PDF** (Reinhard Neder/Ella Schmidt)

15:00 **Wrap up and free discussions** (*coffee break and snack to go*)



We all stay in the INNdependence for the tutorial

Ask if you need something .....

