High-lights of solid state physics at ISOLDE

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- Tracer diffusion: Ag in CdTe
- Transition metal impurities in Si: Fe
- Photoluminescence: nature of the “green band” in ZnO
- Arsenic as an “anti-site” impurity in ZnO
- O and F configurations in High-T_c Hg1201
- Polaron dynamics in Colossal Magneto-Resistive manganites
- Magnetic hyperfine fields of adatoms at surfaces: Cd on Ni

Use of radioactive isotopes in Solid State Physics

- Detect nuclear radiation to quantify impurities:

⇒ radiotracer diffusion

- Decay particles transmit information with atomic resolution:

⇒ Emission Channeling (EC)

⇒ Perturbed Angular Correlation (PAC)

⇒ Mössbauer Spectroscopy (MS)

⇒ Beta Nuclear Magnetic Resonance (β-NMR)

- Identify spectroscopic signals via isotope half life:

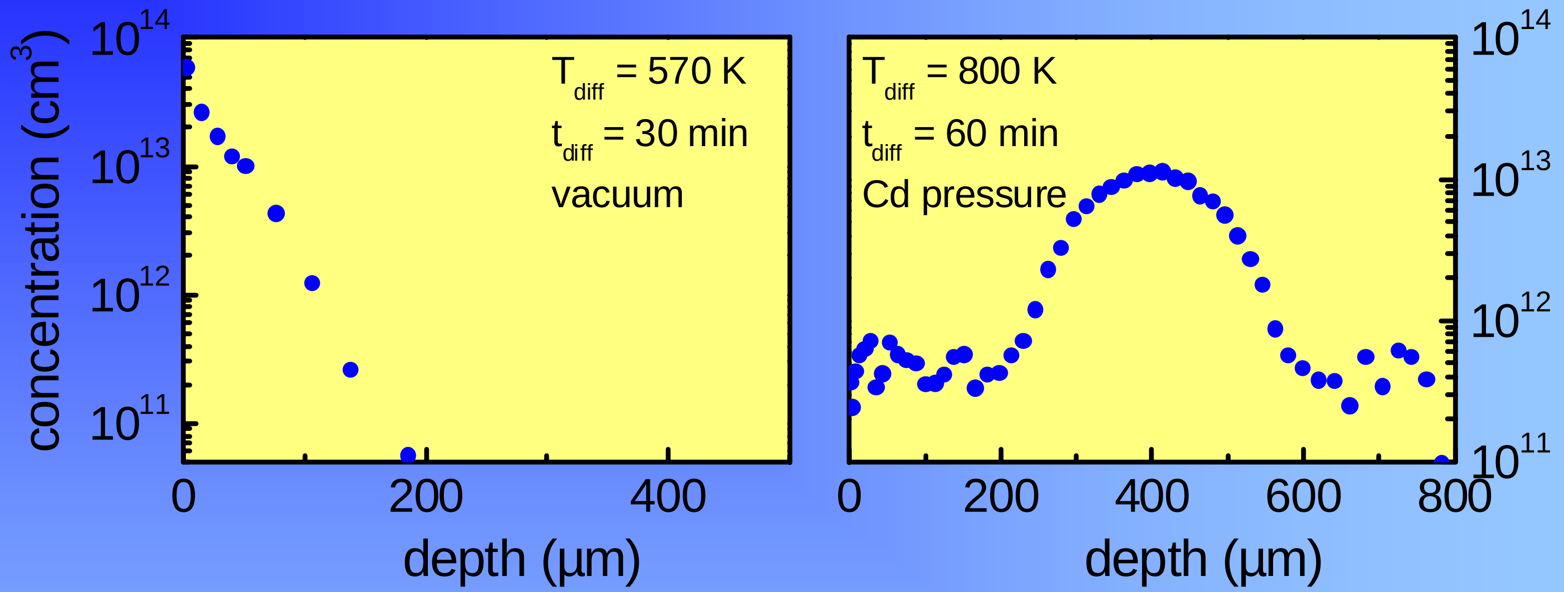
⇒ Photoluminescence (PL)

⇒ Deep Level Transient Spectroscopy (DLTS

⇒ Hall effect

At ISOLDE often several of these methods are used in combination

The “unusual” diffusion of ^{111}Ag in CdTe



“Normal” Gaussian diffusion profile

Very unusual symmetrical diffusion profile

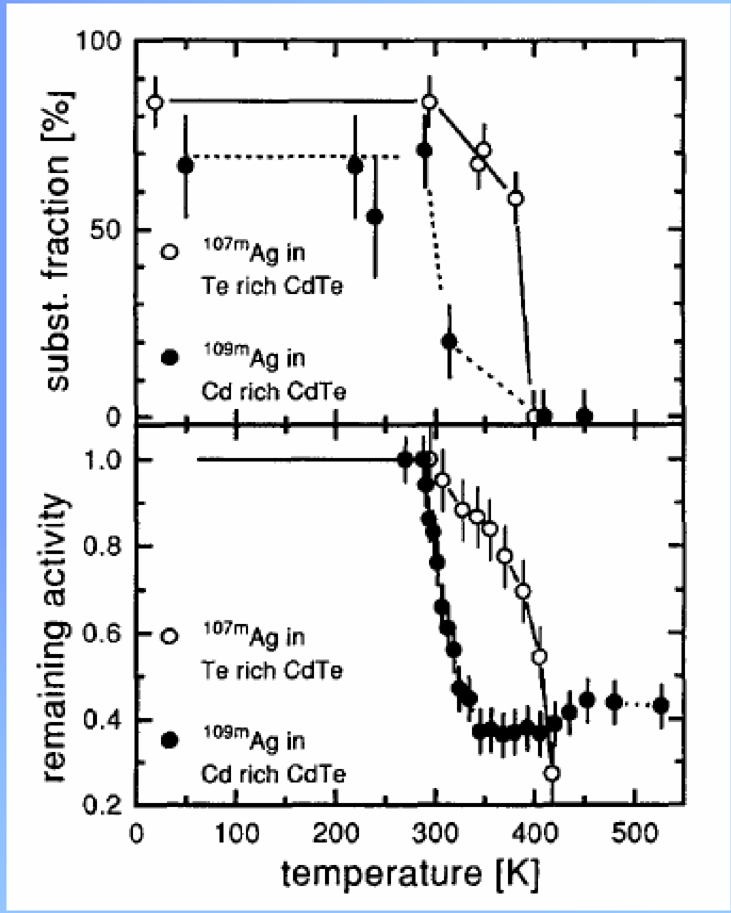
Why?

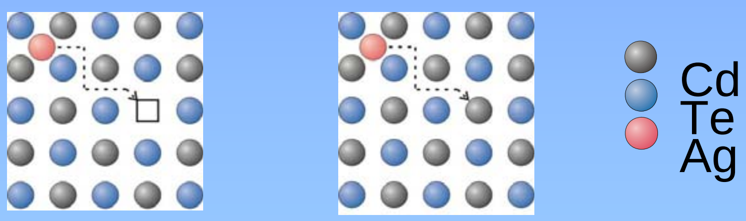
H. Wolf *et al*, Phys. Rev. Lett 94 (2005) 125901

Lattice location of $^{107}Cd \rightarrow {}^{107m}Ag$(40s) and $^{109}Cd \rightarrow {}^{109m}Ag$(44s) in CdTe

Emission Channeling lattice location:

- substitutional Ag_{Cd}
- low stability of Ag_{Cd}
  E_a = 0.92(4)eV
- long-range diffusion
- amount of Ag_{Cd} depends on the Cd stoichiometry



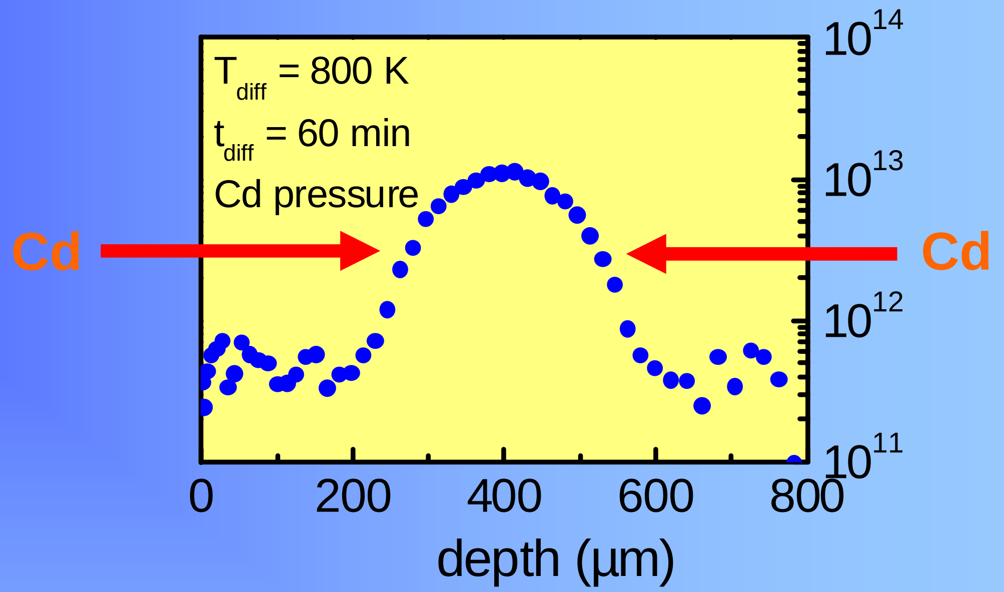


$Ag_i + V_{Cd} \Leftrightarrow Ag_{Cd}$

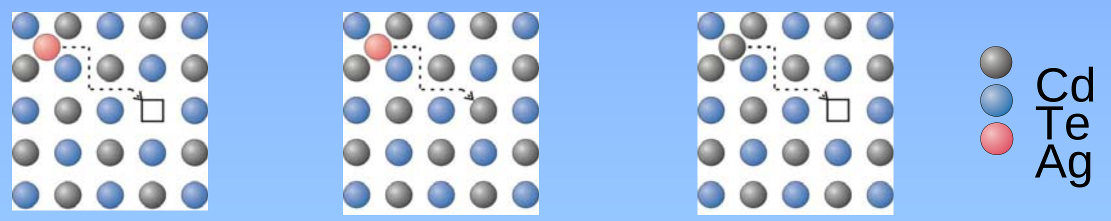
$Ag_i + Cd_S \Leftrightarrow Ag_{Cd} + Cd_i$

Diffusion of ^{111}Ag in CdTe

depletion of Ag in surface regions due to slow indiffusion of Cd
$[Ag_S] \sim [V_{Cd}]$



Symmetrical diffusion profile



$Ag_i + V_{Cd} \Leftrightarrow Ag_{Cd}$

$Ag_i + Cd_S \Leftrightarrow Ag_{Cd} + Cd_i$

$Cd_i + V_{Cd} \Leftrightarrow Cd_S$

H. Wolf *et al*, Phys. Rev. Lett 94 (2005) 125901

International Technology Roadmap for Semiconductors

*Table 32b Starting Materials Technology Requirements—Long Term***

Year of First Product Shipment *Technology Node*	*2008* *70 nm*	*2011* *50 nm*	*2014* *35 nm*
Proposed Year of First Product Shipment, Technology Node (A)	*2008* *60nm*	*2011* *40 nm*	*2014* *30 nm*
DRAM 1/2 Pitch (nm)	70	50	35
New DRAM 1/2 Pitch (nm) (A)	60	40	30
MPU Gate Length (nm)	45	32	22
New MPU/ASIC Gate Length (In Resist) (nm) (A)	45	33	23
General Characteristics * (B,C)			
Wafer diameter (mm)	300	300	450
Edge exclusion (mm)	1	1	1
Front surface particle size (nm), latex sphere equivalent (D)	≥ 35	≥ 25	≥ 17.5
Particles (cm^{-2}) (E,F)	≤ 0.10	≤ 0.10	≤ 0.10
Particles (#/wf)	≤ 73	≤ 72	≤ 165
Critical surface metals (at/cm^2) (G)	≤ 4.2E+9	≤ 3.6E+9	≤ 3.4E+9
Site flatness (nm) (H)			
Oxygen (center point value ± 2.0 ppma) (ASTM '79) (I)			
Polished Wafer *			
Total Allowable Front Surface Light Scattering Defect Density is The Sum of Crystal Originated Pits (COPs) and Particles (see General Cha			
Front surface COPs size (nm), latex sphere equivalent (D)	≥ 35	≥ 25	≥ 18
COPs (cm^{-2}) (J)	≤ 0.10	≤ 0.10	≤ 0.10
Particles (DRAM) (#/wf)	≤ 294	≤ 255	≤ 504
Total bulk Fe (at/cm^3) [K]	< 1×10^{10}	< 1×10^{10}	< 1×10^{10}
Oxidation stacking faults (OSF)			
Oxidation stacking faults (OSF) (MPU) (cm^{-2}) (L)	≤ 0.6	≤ 0.4	≤ 0.2

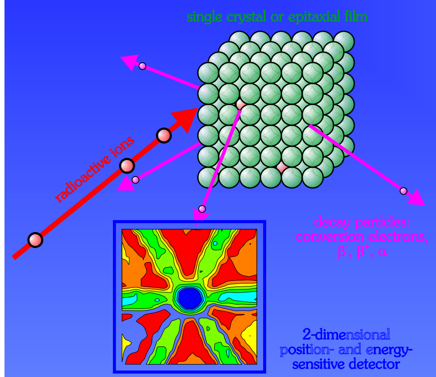
Identify + control Fe in Si below 10^{10} cm^{-3}

Transition metal impurities in Si

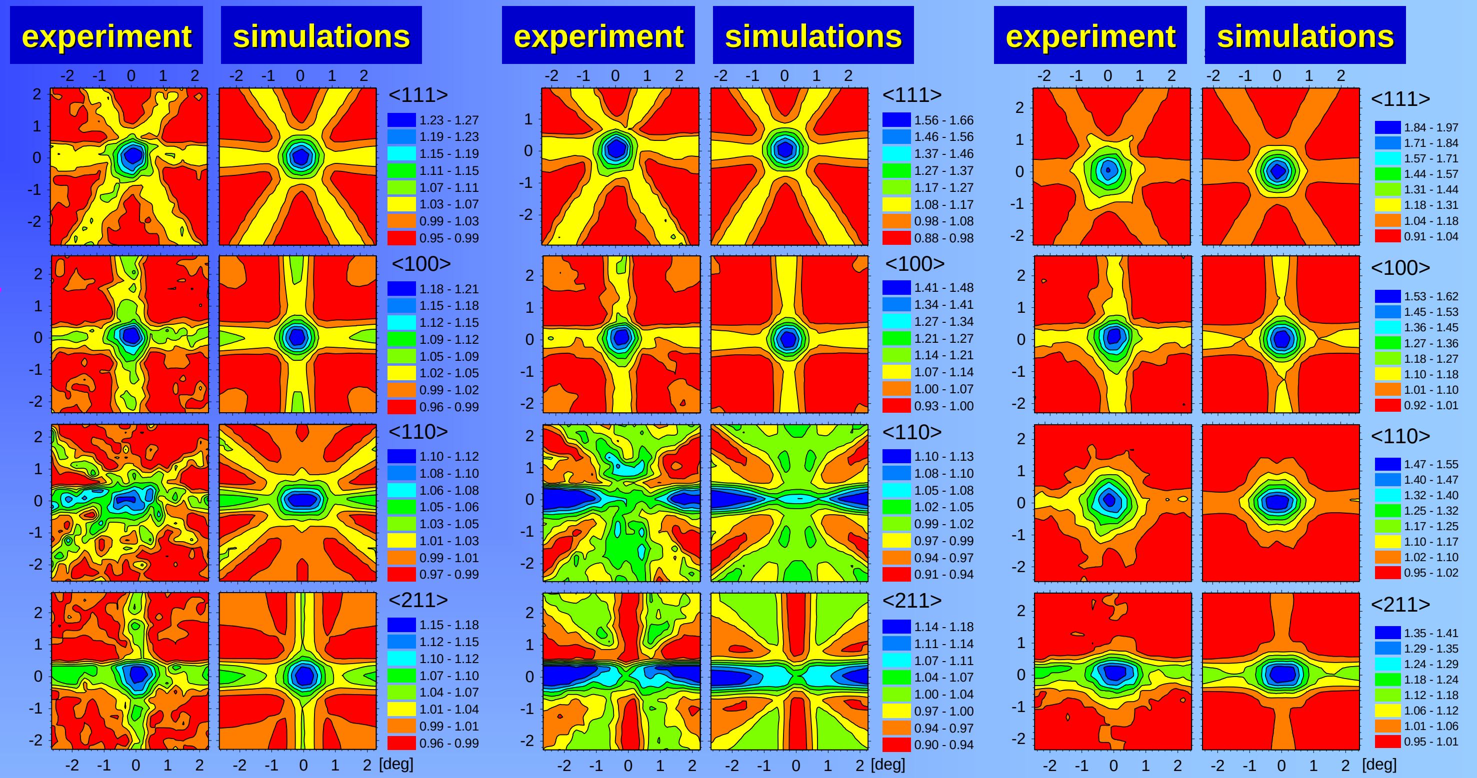
- Fe, Ni, Co, Cu… fast interstitial diffusers
- deep centers
- interact with dopants and change the electrical properties of dopants
- must be gettered away from active region of devices, e.g. by trapping at radiation damage

⇒ investigate properties of Fe in Si by Emission Channeling (EC) and Mössbauer spectroscopy (MS)

Lattice site changes of implanted ^{59}Fe in Si



β⁻ angular emission channeling patterns



RT as-implanted:

mainly displaced substitutional Fe

annealed at *T*=300°C:

mainly tetrahedral interstitial Fe

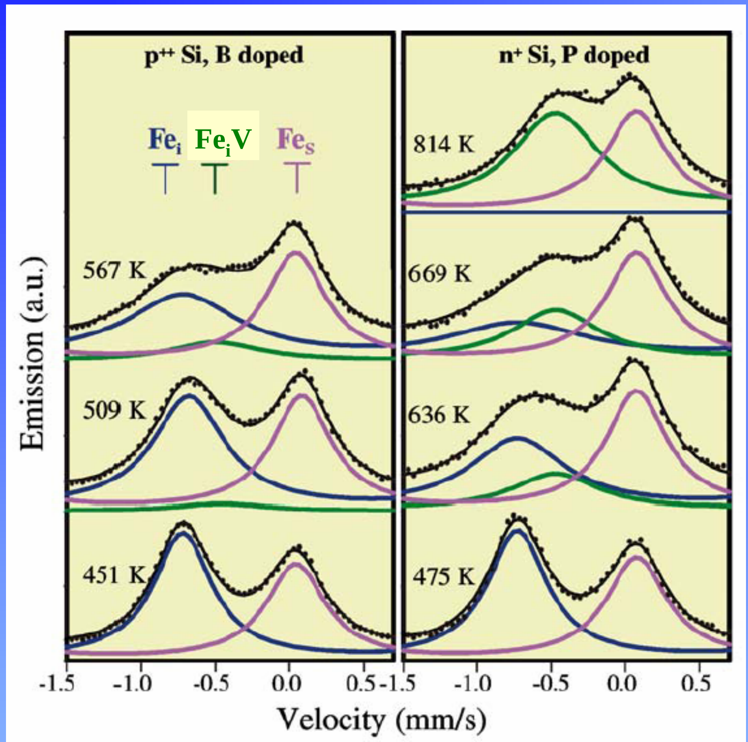
annealed at *T*=800°C:

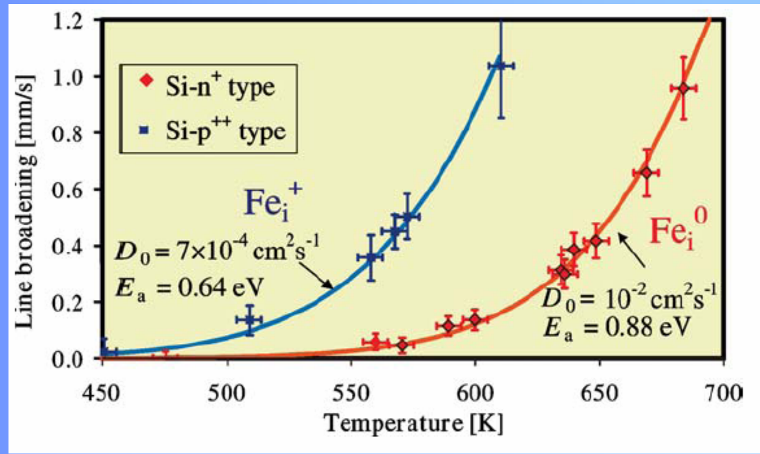
mainly ideal substitutional Fe

- **At least 3 different Fe lattice sites**
- **Following release to interstitial state re-gettering occurs at a different gettering center on ideal substitutional sites**

U. Wahl *et al*, Phys. Rev. B 72 (2005) 014115

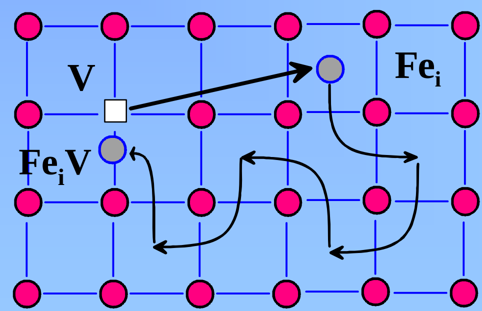
Mössbauer effect from $^{57}Mn \rightarrow {}^{57}Fe$ in Si





- MS line broadening reveals difference in diffusion coefficients of Fe_i^+ and Fe_i^0

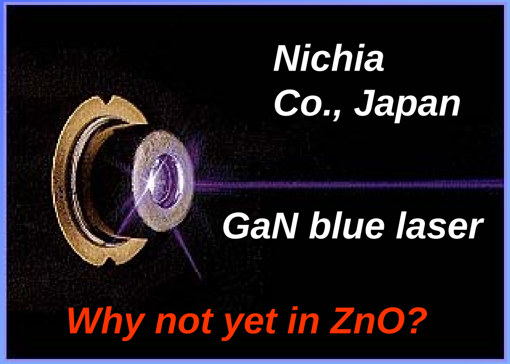
- 4-5 different Fe centers identified
- interstitial Fe seen by EC is probably a (Fe_i-V) complex



H.P. Gunnlaugsson et al, Appl. Phys. Lett. 80 (2002) 2657

Zinc Oxide

- wurtzite semiconductor with band gap of 3.4 eV
- very similar to GaN but with superior optical properties
- large single crystals available

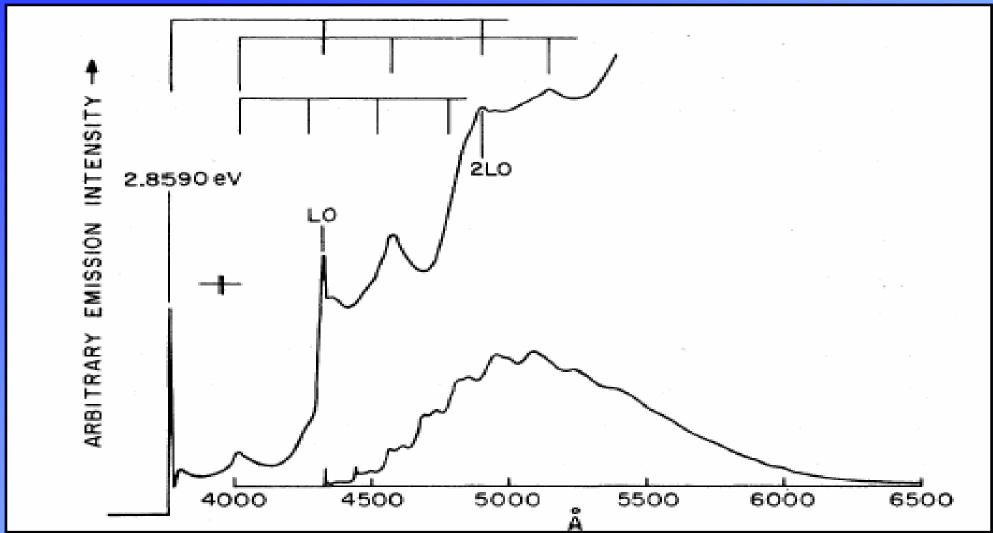


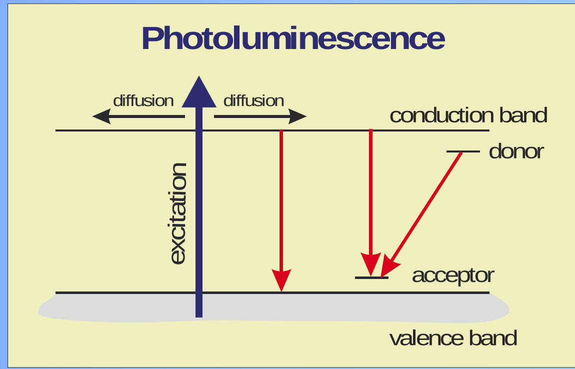
Major problem

- all undoped crystals are *n*-type
  (vacancies, interstitials, other defects, impurities?)
- *p*-doping extremely difficult

Puzzles of the "green band" in ZnO

"Structured" green luminescence band in ZnO





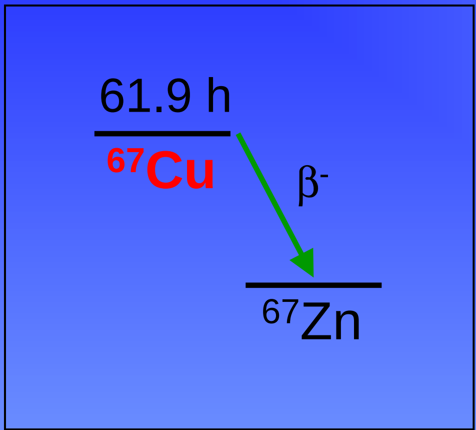
R. Dingle, Phys. Rev. Lett. 23 (1969) 579

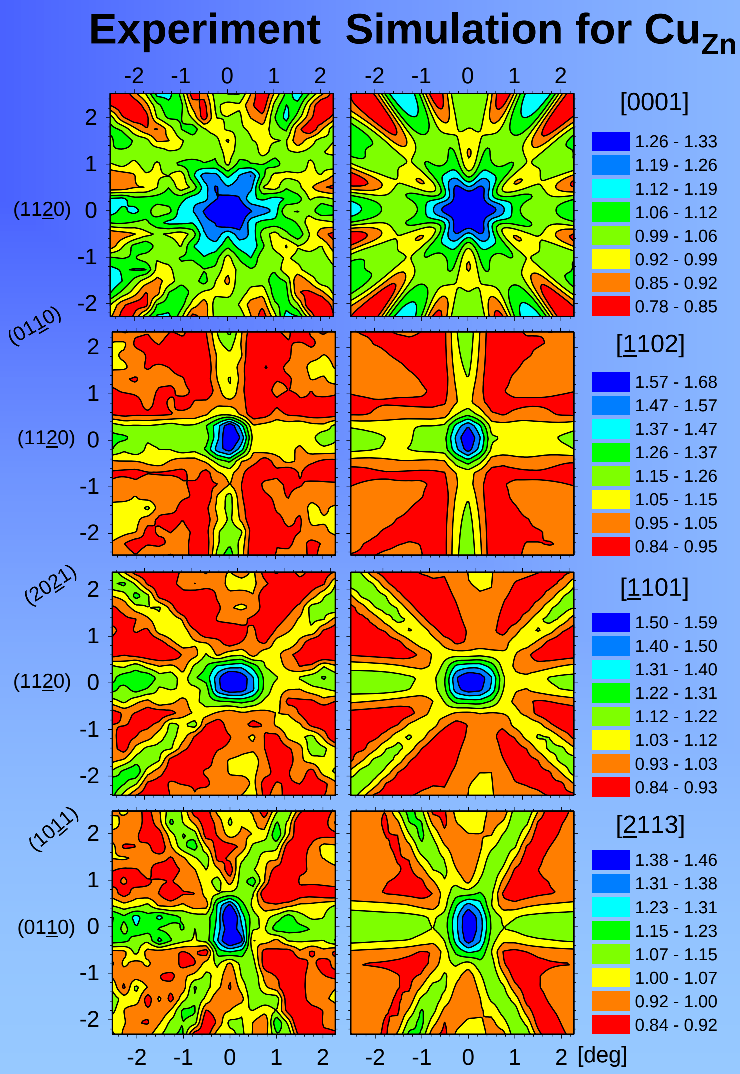
Conflicting explanations for the "green band" in the literature:

- Cu_{Zn} - impurities
- Vacancies (e.g., V_O, V_{Zn})

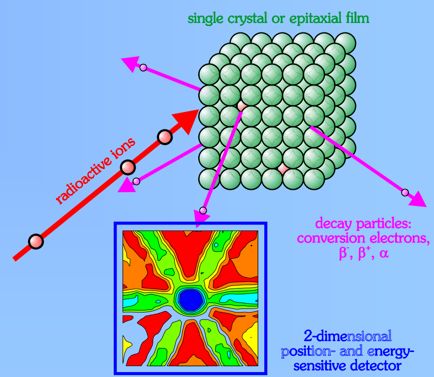
⇒ **investigate properties of Cu in ZnO and nature of green band by emission channeling and PL**

Lattice location of ^{67}Cu→^{67}Zn in ZnO





ISOLDE / CERN:
- 2×10^{13} cm^{-2} at 60 keV
- 200°C, 10 min, vacuum

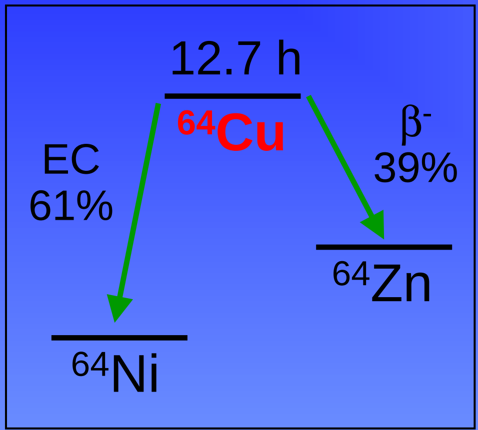


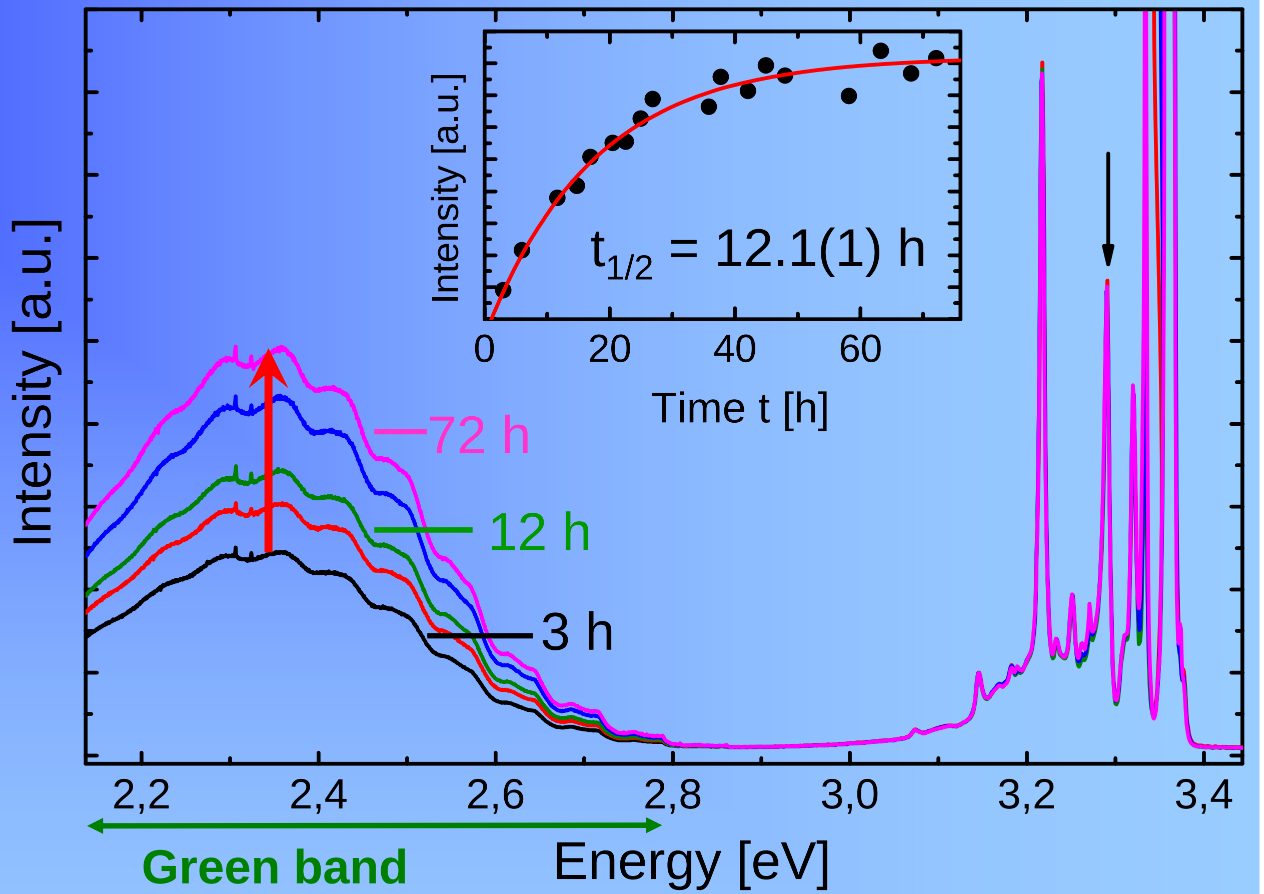
Implanted Cu occupies substitutional Zn sites:

Cu_{Zn} ✓

U. Wahl et al, Phys. Rev. B 69 (2004) 012102

PL-Signals of $^{64}Cu \rightarrow (^{64}Ni, ^{64}Zn)$ in ZnO





ZnO: Green band

Literature

- ~~Cu_{Zn} - impurities~~
- Vacancies

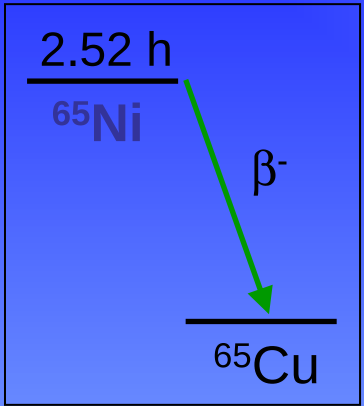
- Ni - impurities ?

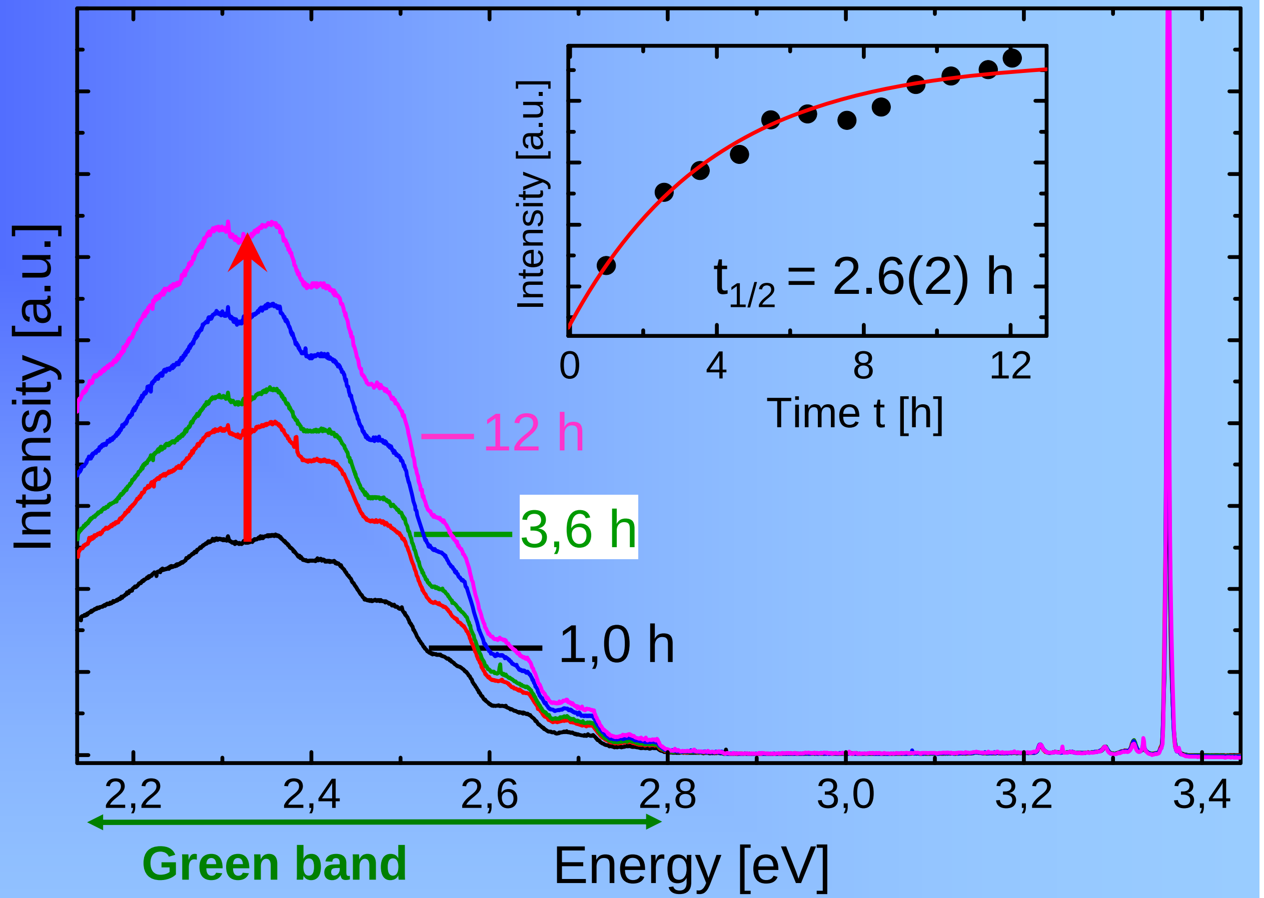
ISOLDE / CERN:

- 5×10^{12} cm^{-2} at 60 keV
- 800°C, 30 min, O_2

T. Agne et al, submitted to Phys. Rev. Lett.

PL-Signals of $^{65}Ni \rightarrow ^{65}Cu$ in ZnO





ZnO: Green band

Literature

- ~~Cu - impurities~~
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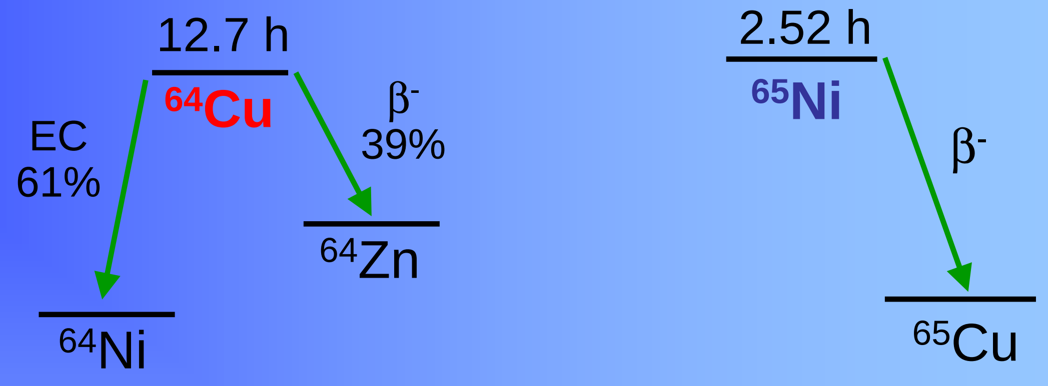
ISOLDE / CERN:

- 5×10^{12} cm^{-2} at 60 keV
- 800°C, 30 min, O_2

T. Agne et al, submitted to Phys. Rev. Lett.

Recoil energies of ^{64}Cu and ^{65}Ni



Recoil energy:

EC - decay
$\rightarrow E_{recoil} = 23.5$ eV

β⁻ - decay
$\rightarrow E_{recoil} \approx 37.7 - 55.7$ eV

Displacement energy in ZnO *: Zn-atoms $E_{displ} = 19$ eV
O-atoms $E_{displ} = 41 - 57$ eV

* D. C. Look, J. W. Hemsky, Phys. Rev. Lett. 82, 2552 (1999)

Both decays produce Zn vacancies:

Green band ↔ Zn vacancies in ZnO

T. Agne et al, submitted to Phys. Rev. Lett.

The difficulties in *p*-type doping of ZnO

Candidates for acceptors:

N, P, <u>As</u>, *Sb*	**Group V on S_O**
Li*, <u>Na</u>, *K*, *Rb	**Group Ia on S_{Zn}**
<u>Cu</u>, <u>Ag</u>	**Group Ib on S_{Zn}**

<u>already studied at ISOLDE</u>

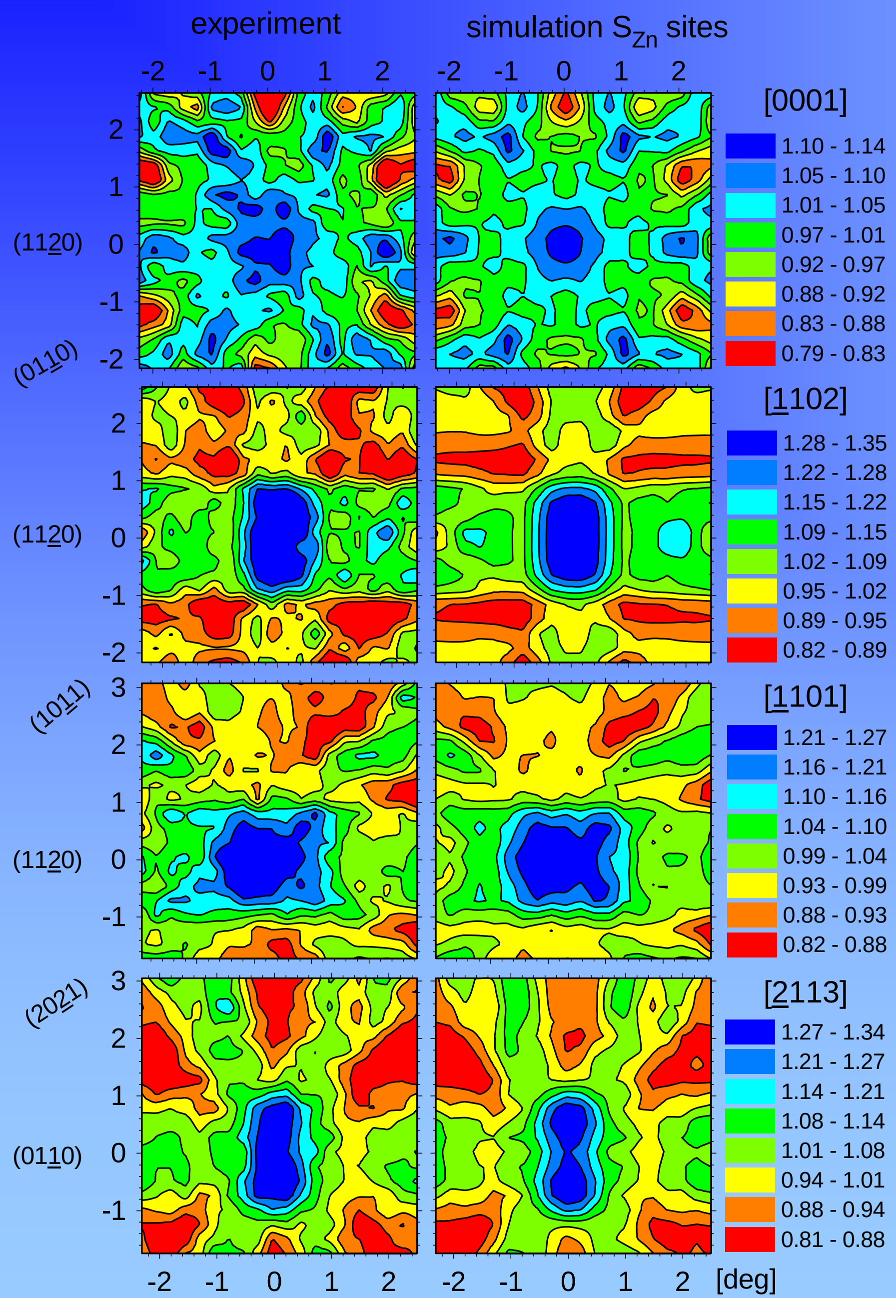
investigations foreseen

<u>Example</u>:

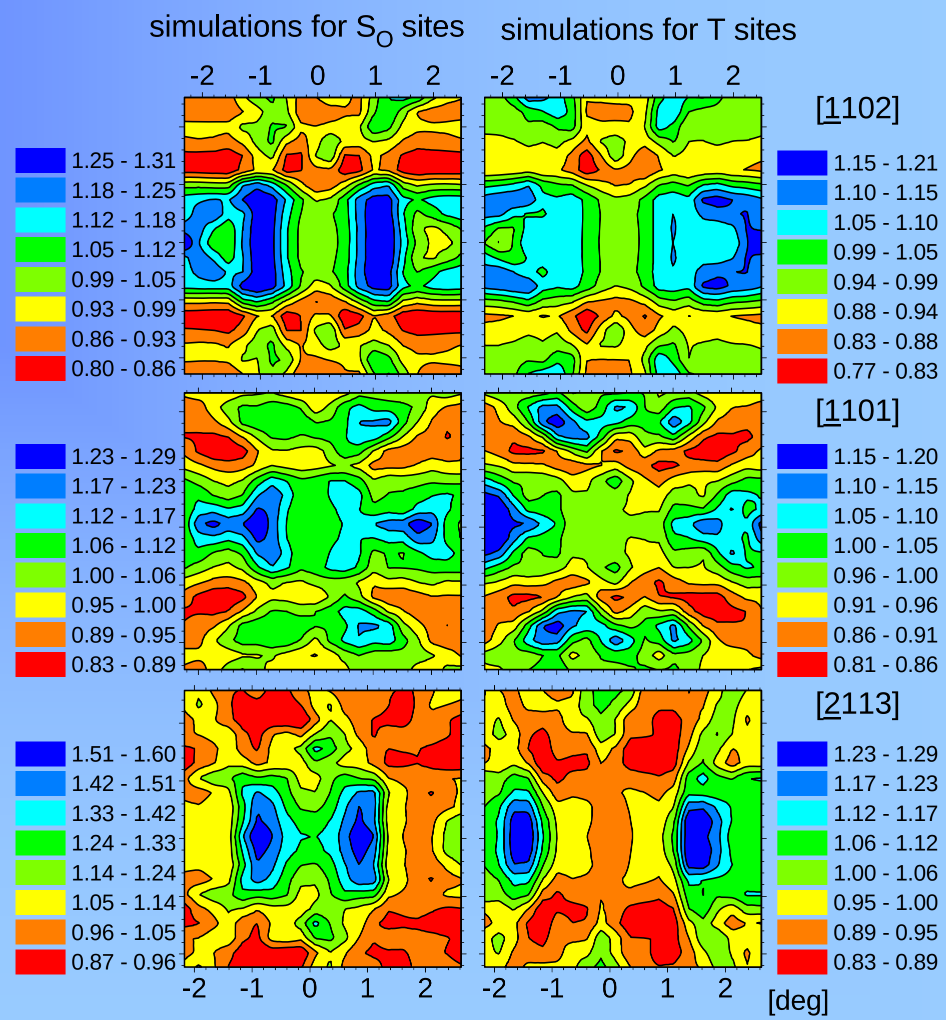
Is As a suitable acceptor in ZnO?

Maybe, but it does not like to occupy O sites but prefers Zn sites!

^{73}As as an "anti-site" impurity in ZnO



Only patterns for S_{Zn} fit the experimental results!

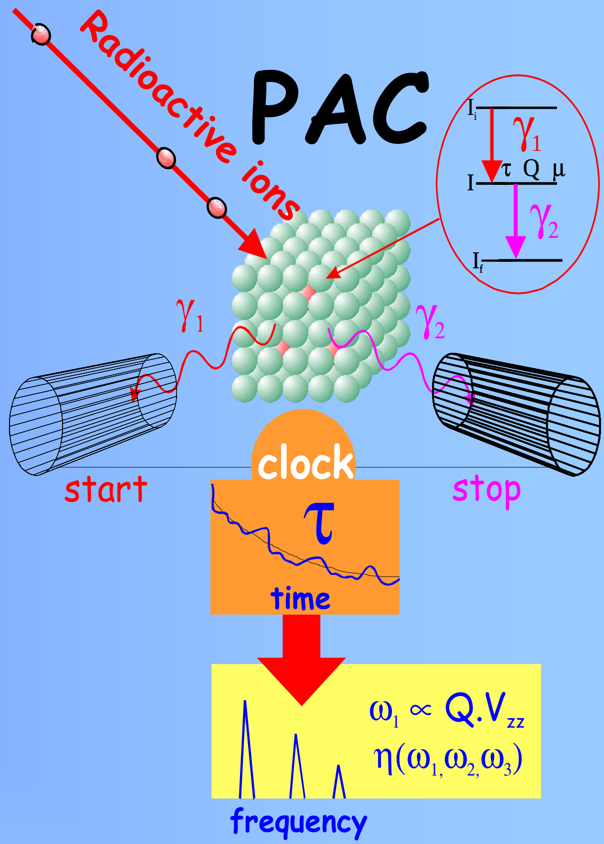


U. Wahl *et al*, in print, Phys. Rev. Lett. (2005)

High-T_c superconductors

- Superconductivity and its T_c critically influenced by the charge that O^{2-} doping introduces in the superconducting CuO_2 planes
- Twice the number of F^- introduce the same charge doping

⇒ investigate atomistic configurations of O^{2-} and F^- dopants by means of electrical field gradient (EFG) it causes on PAC probe atom ^{199m}Hg



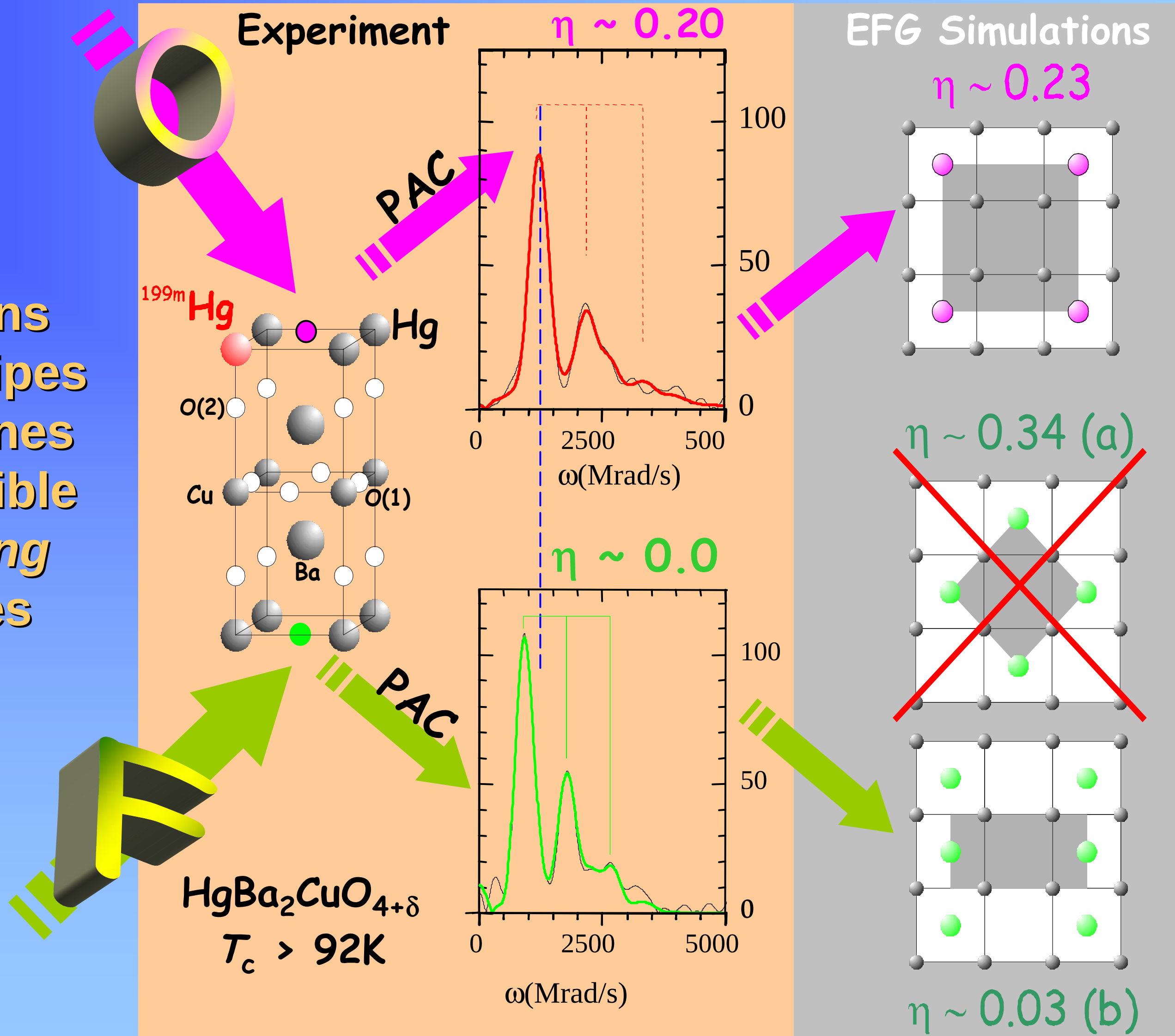
Electric Field Gradient

⇔

dopant configuration fingerprint

Oxygen & Fluorine Configurations in Hg1201 (High-T_c)

- **In contrast to O, F orders in small atomistic stripes**
- **Local deformations and atomistic stripes in the doping planes are <u>NOT</u> responsible for *charge ordering* at the CuO_2 planes**



J.G. Correia *et al*, in press, Phys. Rev. B (2005)

Colossal Magnetoresistive Manganites

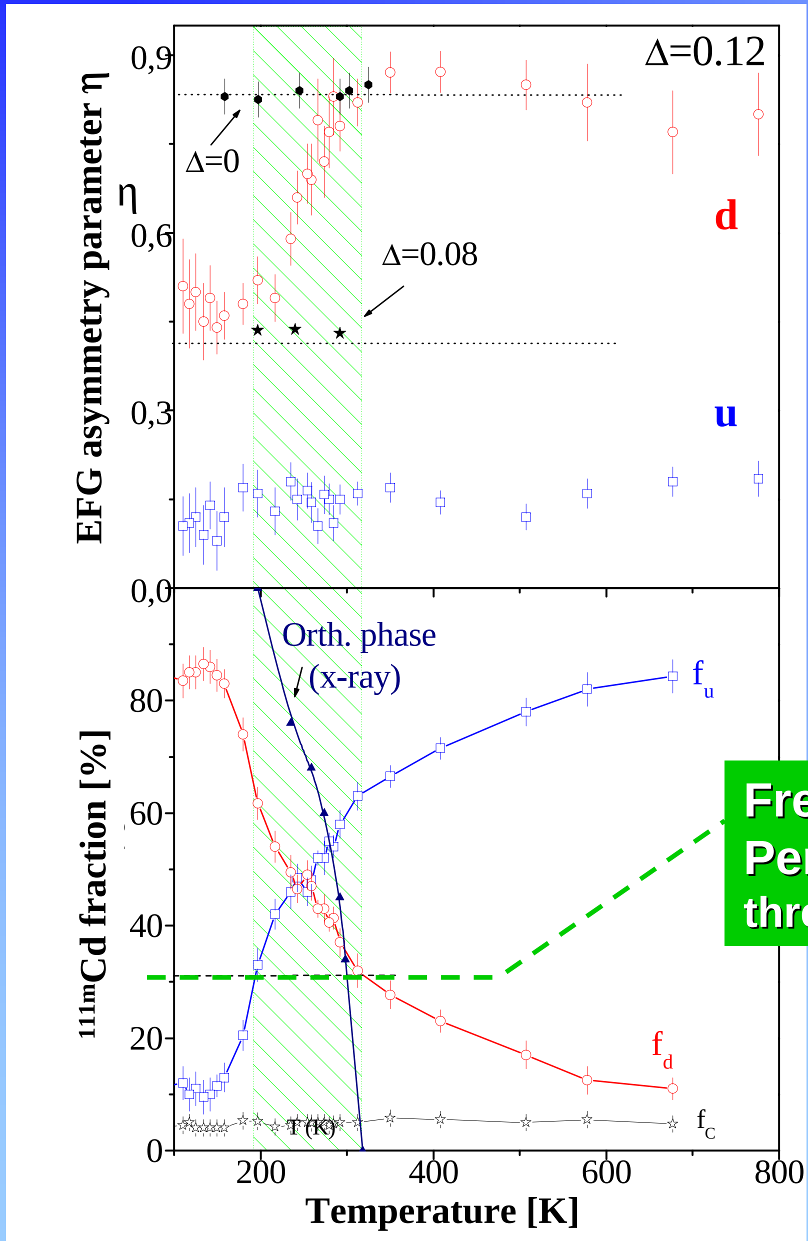
Strong coupling of
spin, **charge**, **orbital** and **lattice degrees of freedom**

Complex multi-scale world with:

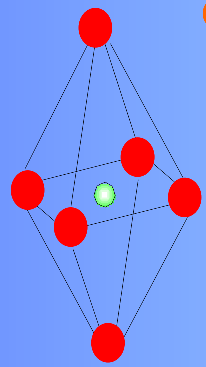
Intrinsic inhomogeneities
Clusters and stripes (charge, spin and structure)
Unconventional phase transitions
Charge-coupled lattice deformations: Polarons

⇒ use ^{111m}Cd impurities as local observers of the nature of structural phase transitions by means of PAC

Unconventional phase transitions as seen by ^{111m}Cd in $LaMnO_{3.12}$

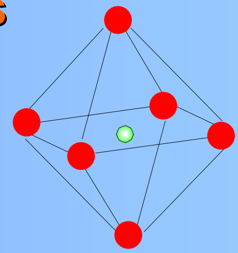


Two main local $^{111m}Cd_{La}$ environments



EFG d

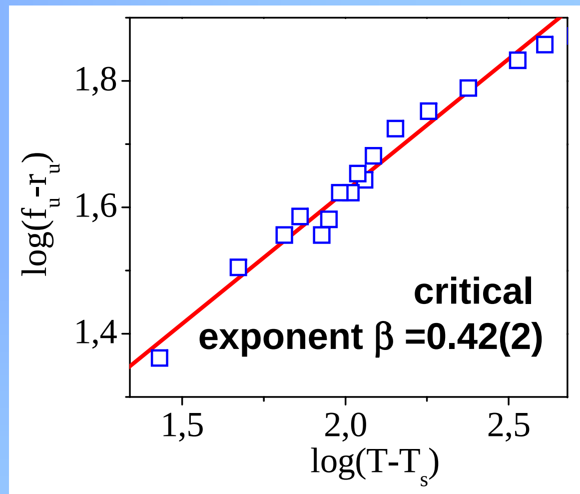
Strong Jahn-Teller Distortion



EFG u

Undistorted

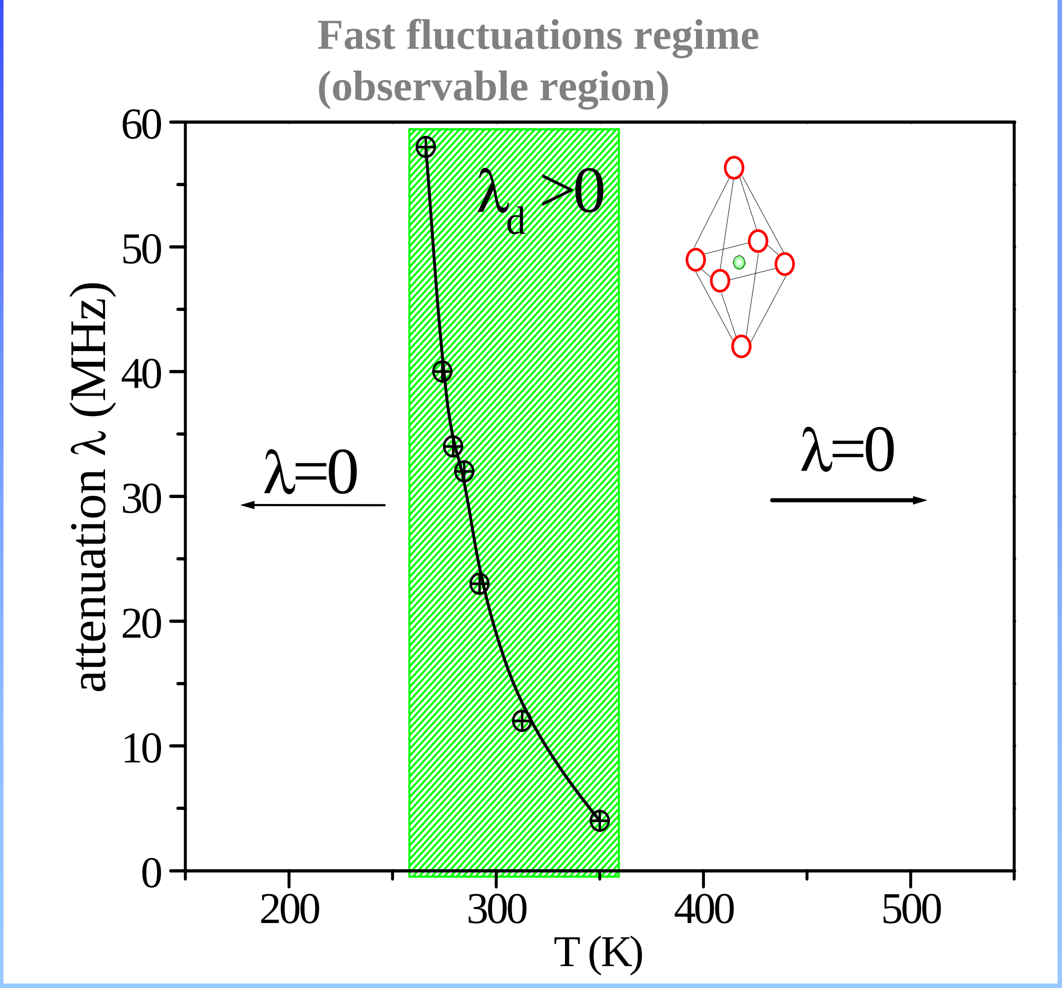
Free Percolation threshold: 31%

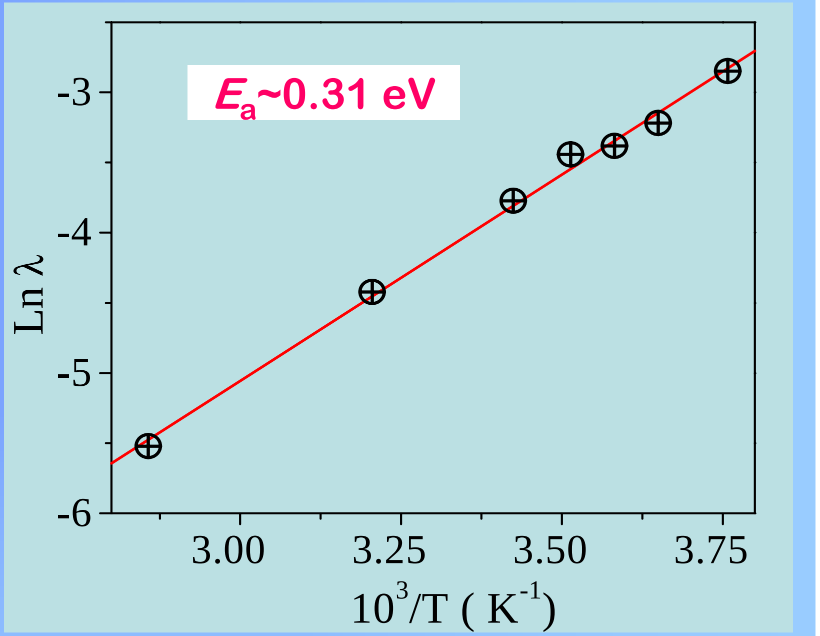


A.M.L. Lopes et al, submitted to Phys. Rev. Lett.

^{111m}Cd in $LaMnO_{3.12}$: polaron dynamics

Dynamic Jahn-Teller distortions related to polaron diffusion give rise to EFG fluctuations/attenuation





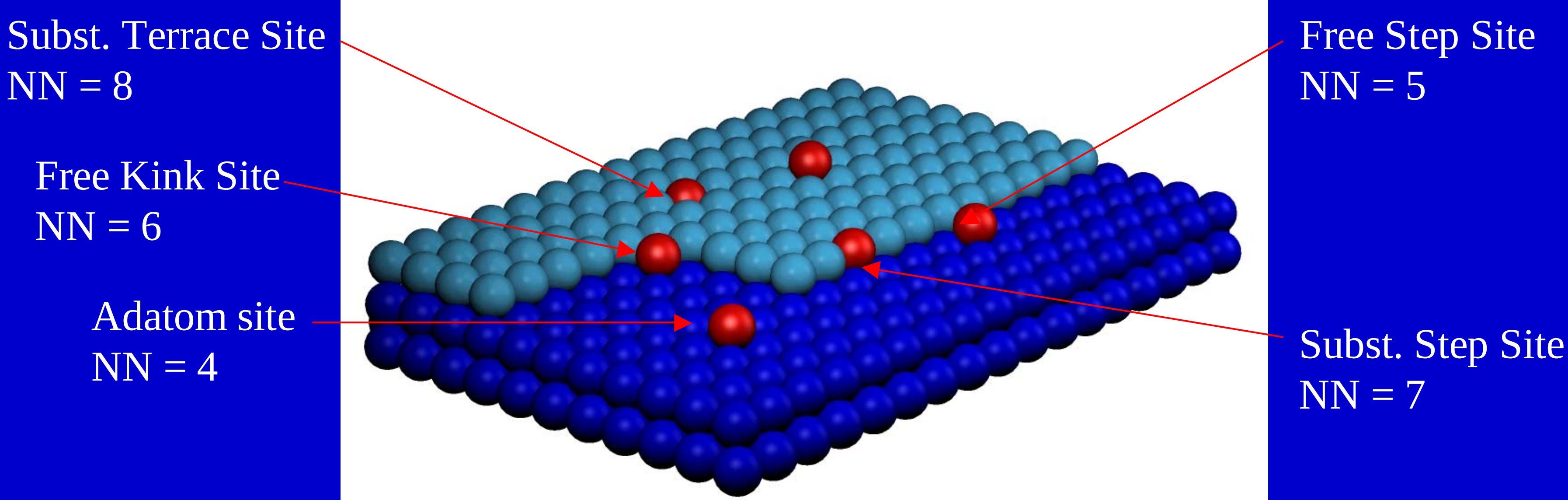
- **Thermally activated polaron dynamics**
- **Hopping energy E_a~0.31 eV**

A.M.L. Lopes et al, submitted to Phys. Rev. Lett.

Magnetism on surfaces

Impurity Atoms at Various Sites on a Surface (001)

^{111}Cd Probe on Ni(001)



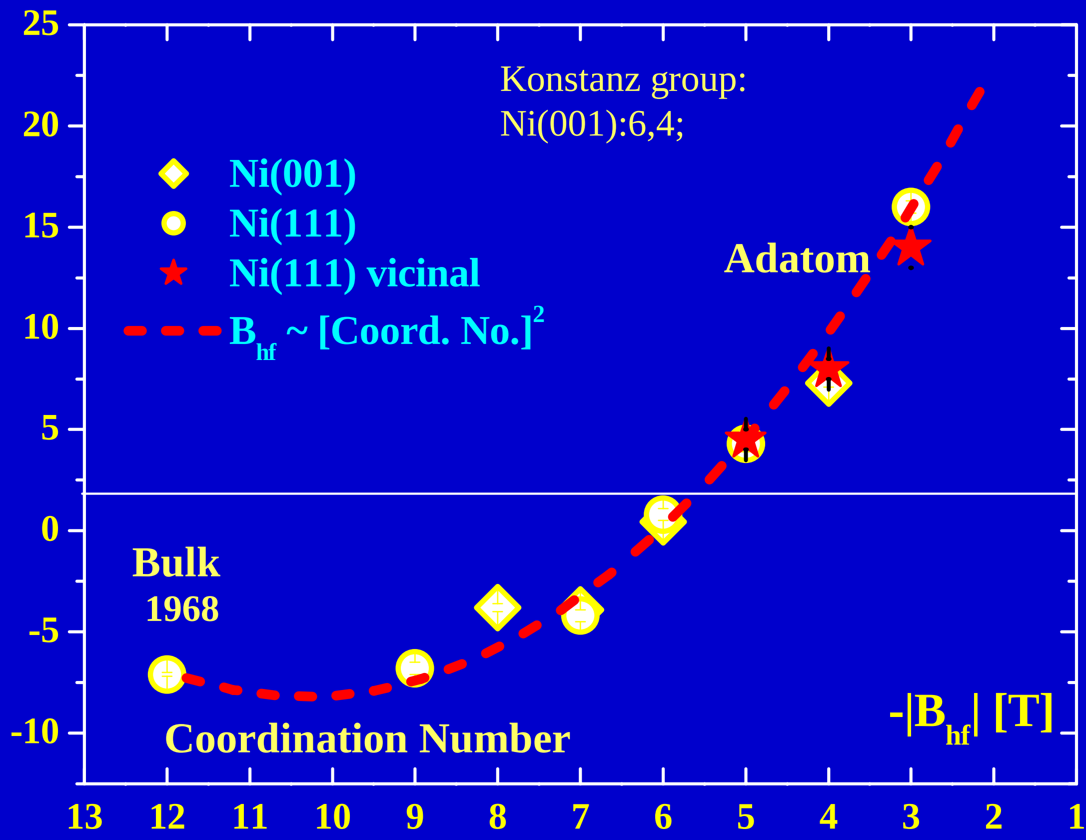
Different adatom sites can be prepared via deposition and anneal temperature

⇒ allows systematic studies of magnetic hyperfine fields B_{HF} at different sites by means of PAC

B_{HF} parabolic function of coordination number

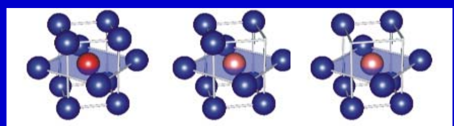
K. Potzger et al, Phys. Rev. Lett. 88 (2002) 247201

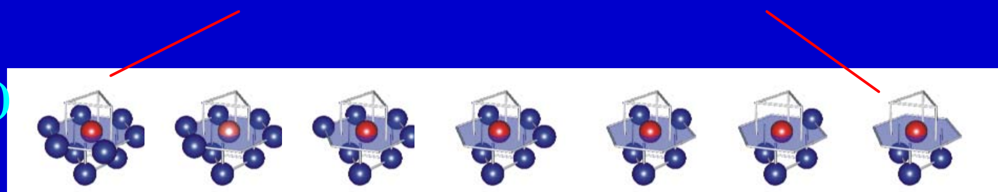
Theory: Mavropoulos et al. PRL **81**, 1506 (1998)

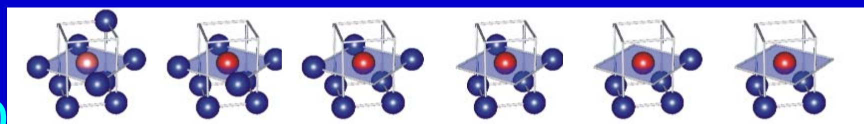


Magnetic Hyperfine Fields at ^{111}Cd on Ni Surfaces

Ni(111)







Ni(001)

Solid state physics at ISOLDE covers a wide range of materials:

- **Semiconductors:**

  Si, Ge, SiGe, diamond,
  III-V, nitrides, II-VI, ZnO…

  electrical doping, transition metals,
  rare earths, H,
  diluted magnetic semiconductors

- **High-T_c superconductors and perovskites**
- **Magnetism (manganites, CMR)**
- **Low dimensional systems:**
  surfaces, interfaces, multilayers

ISOLDE's strength:
the variety of different experimental methods that can be combined to study these materials

Thanks to

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