Untersuchung von Punktdefekten in ZnO mit Positronen

G. Brauer

[1]Institut für Ionenstrahlphysik und Materialforschung, Forschungszentrum Dresden-Rossendorf, Postfach 51 01 19, 01314 Dresden

Miniworkshop
„Die Positronenannihilation in der modernen Werkstoff-Forschung“
02.April 2008
Forschungszentrum Dresden – Rossendorf

General remarks

- ZnO is a wide band gap semiconductor (~ 3.4 eV at 300 K)

- ZnO is a promising material for:

  * visible + UV light emission

  * detectors / sensors

  * high-temperature electronics

- lattice defects control optical and electrical properties

- structure / configuration of lattice defects in ZnO is widely unknown

  * native defects may exist

  * two sublattices exist

  * charge states of defects are possible

  PAS may help to identify these defects !!!

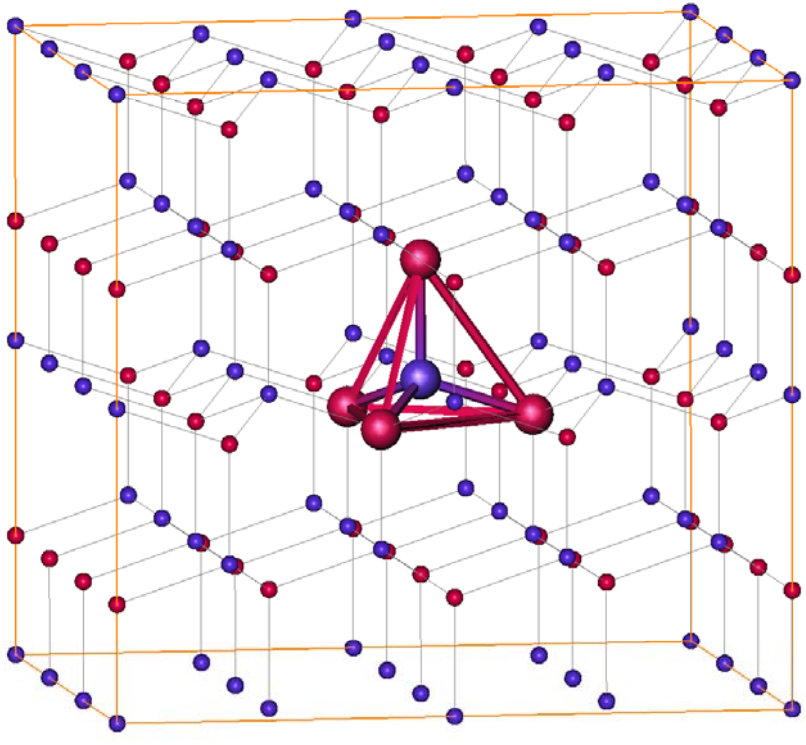
- ZnO high quality single crystals are commercially available now:

  * hydrothermal growth (HTG)

  * pressurized melt growth (MG)

TECHNOLOGICAL APPLICATIONS also require the use of:

- ZnO films (special preparations)
- ZnO nanorods (special preparations)
- ZnO tetrapods (special preparations)



ZnO perfect lattice (hexagonal, Wurtzite) together with the identified ZnO_4 ‚structure building unit' (red/blue tetrahedron)

In red color: oxygen In blue color: zinc

Positron lifetime calculations

The positron lifetime τ is

a unique value for a given materials state (bulk, or defect)
can be calculated from the general formula:

$$1/\tau = \pi r_0^2 c \int n_-(\mathbf{r})\, n_+(\mathbf{r})\, \gamma[n_-(\mathbf{r})]\, d\mathbf{r}$$

- r_0 – classical electron radius
- c – speed of light
- n_- (n_+) – electron (positron) density
- γ – enhancement factor (depends on n_-), to account for electron-positron interaction

First comprehensive calculations for ZnO:

G. Brauer W. Anwand, W. Skorupa, J. Kuriplach, O. Melikhova, C. Moisson, H. von Wenckstern, H. Schmidt, M. Lorenz, M. Grundmann
Phys. Rev. B 74 (2006) 045208

Enhancement factor used – see for details:
- Boroński and Nieminen, PRB **34** (1986) 3820
- correction for incomplete positron screening (ε_∞=4.0) after Puska et al., PRB **39** (1989) 7666

- electron density comes from the superposition of atomic densities (ATSUP)
- positron Schrödinger equation solved using the ATSUP method

  $n_+=|\psi_+|^2$ (with ψ_+ being the positron ground state)
  - Puska and Nieminen, J. Phys. F: Metal. Phys. **13** (1983) 333
  - A.P. Seitsonen et al., Phys. Rev. B **51**, 14057 (1995)
- relaxed atomic positions obtained by minimizing the total energy
  - plane wave pseudopotential code VASP (=Vienna ab initio simulation package) used
  - Kresse and Hafner, PRB **47** (1993) 558.

Positron lifetimes in ZnO (THEORY)

 # Lattice relaxations, positron lifetimes and positron binding energies to defects in ZnO

Defects relaxed using VASP
Positron calculations by ATSUP (numbers given in brackets in the table)
Relaxations (Zn 1nn; O 1nn) are given in units of ZnO lattice constant
Two different types of enhancement factor used: "Boronski-Nieminen (BN)" , and "Gradient Correction (GC)"

defect	relaxations (%)	ATSUP-BN		ATSUP-GC	
		lifetime (ps)	energy (eV)	lifetime (ps)	energy (eV)
bulk	—; —	159	—	176	—
V_O	+4.6; —	159 (160)	0.01 (0.02)	177 (178)	0.01 (0.02)
V_{Zn}	—; –9.7	229 (194)	0.60 (0.35)	257 (211)	0.50 (0.22)
$V_{Zn+O}(1)$	–17.1; –11.4	286 (224)	1.23 (0.61)	327 (250)	1.19 (0.54)
$V_{Zn+O}(2)$	–14.6; –7.5	276 (223)	1.10 (0.61)	313 (250)	1.06 (0.54)

 # Adjustment from experiment required to choose 'the best' enhancement factor

 # Our experimental value (CERMET 2002, melt grown crystals): τ_b **= (151 ± 2) ps**

G. Brauer W. Anwand, W. Skorupa, J. Kuriplach, O. Melikhova, C. Moisson, H. von Wenckstern, H. Schmidt, M. Lorenz, M. Grundmann
Phys. Rev. B 74 (2006) 045208

 # Conclusion: BN approach is the better choice for calculations in ZnO

Positron lifetimes in ZnO (experimental situation)

Until 2002:

High quality ZnO single crystals are almost unavailable on the market
Several types of ZnO materials were studied by positron lifetime technique in the literature
Given τ_b values vary with origin of sample, pointing to the influence of grown-in defects, i.e. method of growth matters !

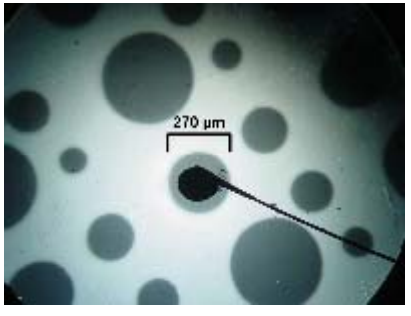
2003 – 2006:

One pair of ZnO single crystals from Cermet is available to us for investigations
Results are summarised in two major publications:

G. Brauer, W. Anwand, W. Skorupa, J. Kuriplach, O. Melikhova, C. Moisson, H. von Wenckstern, H. Schmidt, M. Lorenz, M. Grundmann
Defects in virgin and N+ implanted ZnO single crystals studied by positron annihilation, Hall effect and deep level transient spectroscopy
Phys. Rev. B 74 (2006) 045208 (10 pp)

H. von Wenckstern, R. Pickenhain, H. Schmidt, M. Brandt, G. Biehne, M. Lorenz, M. Grundmann, G. Brauer
Deep acceptor states in ZnO single crystals
Appl. Phys. Lett. 89 (2006) 092122 (3 pp)

First bipolar diode of ZnO demonstrated in Europe !
(p-type doping only rudimentary demonstrated in USA and Japan until **August 2006**)



Transparent pn-diode, illuminated from the back, with Pd contacts (one bonded)

2004:

New high quality single crystals became available from MaTecK

2005 – 2006:

Our investigations reveal that hydrogen is attached to open volume defects in ZnO
Summary of the experimental situation published:

G. Brauer, J. Kuriplach, J. Cizek, W. Anwand, O. Melikhova, I. Prochazka, W. Skorupa
Positron lifetimes in ZnO single crystals
Vacuum 81 (2007) 1314-1317

2006 – now:

More systematic investigation of several ZnO single crystals
Investigation of several technologically important ZnO materials (thin films, nanorods)

Positron lifetimes in ZnO (experimental results)

Cermet (2002): melt grown (MG) single crystals

Positron lifetime measurements at Rossendorf (FWHM: 250 ps; 10^6 events)

Free fitting of the results gives:

τ_1 = (93 ± 3) ps, τ_2 = (257 ± 2) ps, I_1 = (39.9 ± 0.7) %, and I_2 = (60.1 ± 0.7) %

One-state trapping model gives:

τ_b = (151 ± 2) ps

 # Conclusion:

τ_2 represents the neutral Zn+O divacancy (concentration: ~3.7 × 10^{17} cm^{-3})

MaTecK (2004): hydrothermally grown (HTG) single crystals

Positron lifetime measurements at Prague (FWHM: 160 ps; 10^7 events)

Free fitting of the results gives:

τ = (182.1 ± 0.4) ps, I = 100 % saturation trapping !!!

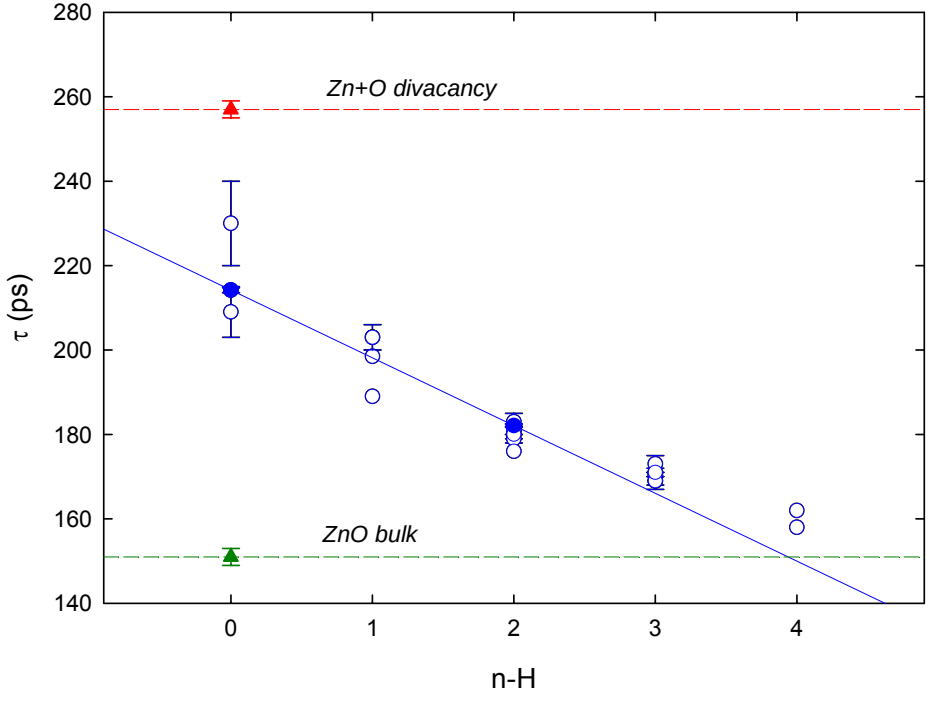
 # Conclusion:

τ is representing a defect being smaller than the Zn vacancy (rigid lattice:194 ps; relaxed lattice: 229 ps - from calculations)

G. Brauer, W. Anwand, W. Skorupa, J. Kuriplach, O. Melikhova, J. Cizek, I. Prochazka, C. Moisson, H. von Wenckstern, H. Schmidt, M. Lorenz, M. Grundmann
Comparative characterization of differently grown ZnO single crystals by positron annihilation and Hall effect
Superlattices and Microstructures 42 (2007) 259-264

Positron lifetimes in ZnO (new ideas about defects)

Collection and display of all available shorter positron lifetime data from the literature in one diagram



Full symbols represent our own ZnO data from Cermet 2002 and MaTecK 2004.

seemingly four well-separated lifetime levels exist between the bulk and Zn vacancy (V_{Zn}) lifetimes

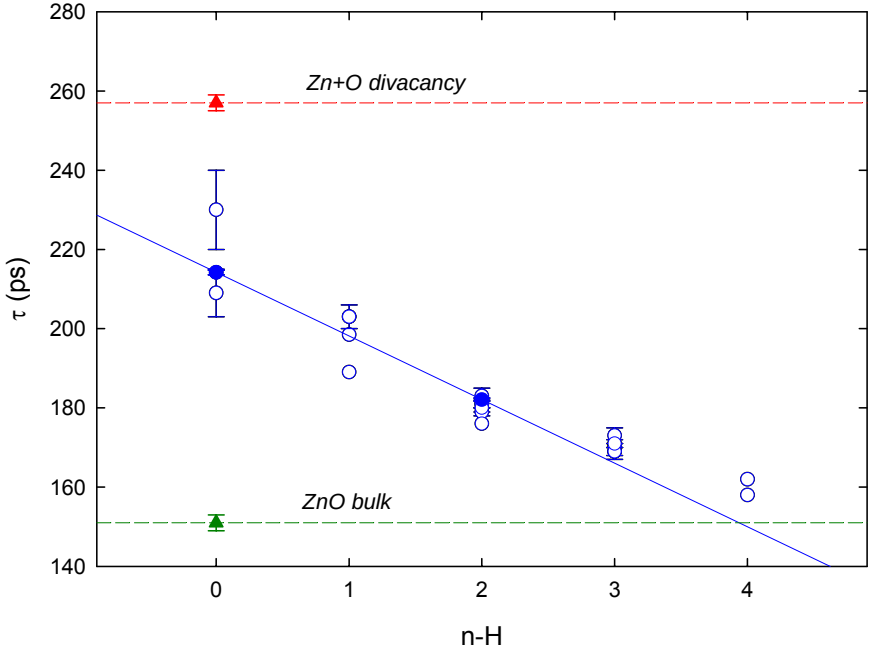
most materials are hydrothermally grown

the decorating impurity of a Zn vacancy is most probably hydrogen

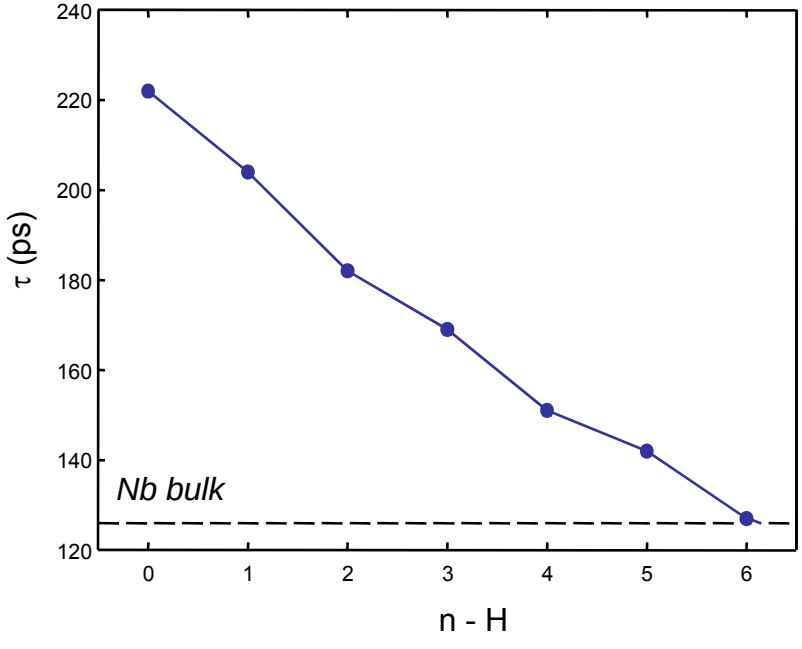
Positron lifetimes in ZnO (new ideas about defects)

Decoration of a vacancy by hydrogen

ZnO - ???



Nb:H – yes, well-known

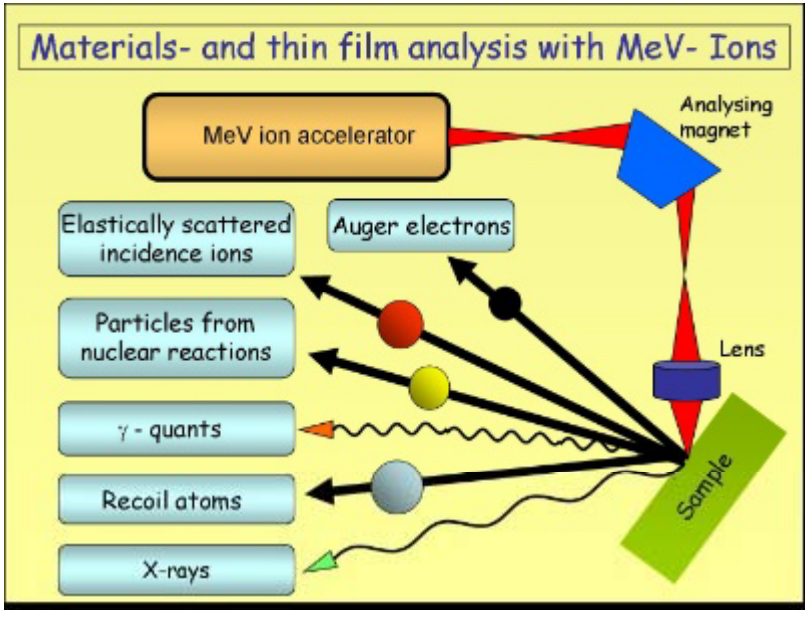


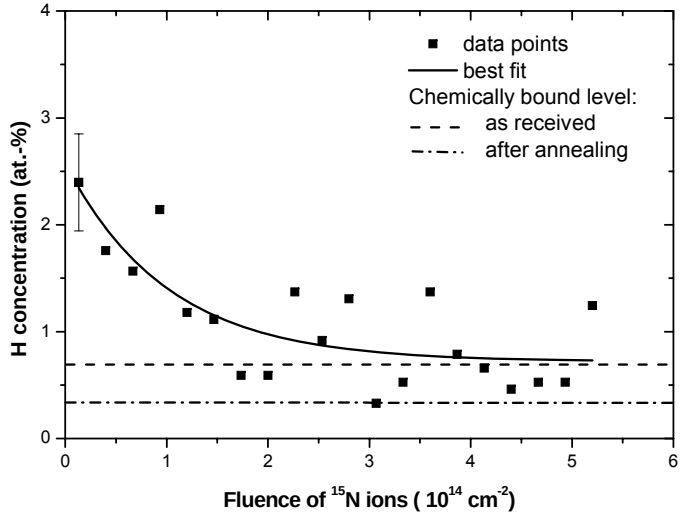
vacancy – H complexes in Nb

J. Cizek, I. Prochazka, F. Becvar, R. Kuzel, M. Cieslar, G. Brauer, W. Anwand, R. Kirchheim, A. Pundt
Hydrogen-induced defects in bulk niobium
Phys. Rev. B 69 (**2004**) 224106 (13 pp)

Positron lifetimes in ZnO (more systematic studies)

Estimation of H content of the samples by Nuclear Reaction Analysis at Rossendorf





Nuclear Reaction Analysis

$^{15}N + {}^{1}H \rightarrow {}^{12}C + {}^{4}He + \gamma$-rays

bombardment energy of ^{15}N: 6.64 MeV
reaction g-rays energy: 4.43 Mev
detection limit: 0.02 at.-%

MaTecK 2004 sample (at 100 nm depth):

Virgin state: 1.9 at.-% unbound H; 0.7 at.-% chemically bound H
Annealed (500 °C, 30 min, air): 0.3 at.-% chemically bound H

Positron lifetimes in ZnO (more systematic studies)

 # chemical analysis of all available as-grown samples by ICP-MS (Inductively Coupled Plasma Source – Mass Spectrometry) **and NRA too**

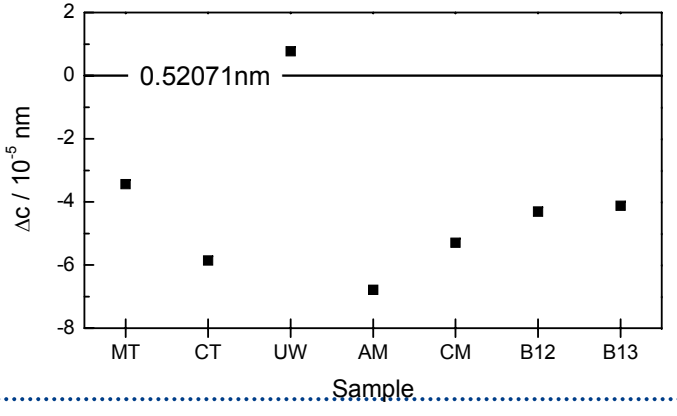
 # sophisticated X-ray diffraction studies (detection of internal stresses and mosaic structures)

 # investigation of a variety of ZnO single crystals

HTG (MaTecK 2004; MaTecK 2006; University Wafers; Altramet); **MG** (Cermet 2006; IKZ12+13)

Sample	Li	Mg	Al	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Ga	Rb	Sr	Zr	Mo	Ag	Cd	In	Sn	Sb	Te	Pt	Pb	Bi	H-b	H-u	H-a
MT-04	0.33	3.32		0.71	0.07	0.07	0.07	0.61	0.03	6.93	3.09	0.06					0.14	2.05	0.03				0.03	0.07	0.04	0.7	1.9	0.3
MT-06			80.6				0.27		0.12	1.11	0.95			0.09				0.03								0.3		0.3
UW	5.37					0.01	0.30		0.04	3.67	0.43	0.54	0.01			0.00	0.43	0.17	0.01		0.00			0.01		0.8	1.7	
AM	6.25					0.01	0.65		0.11	0.40	0.37	0.56	0.01		0.29	0.00	0.16	0.11	0.00	0.11	0.00	0.04		0.01		0.5		
CT			19.4			0.25				0.80	0.69	1.08	0.02				0.16	1.89						0.04		0.3		0.3
CM						0.01				0.22	0.34	0.43	0.01			0.00	0.16	0.17	1.54	0.02	0.00	0.04		0.09		0.5		
B12						0.01			0.03	0.12	0.65	0.60	0.01		0.09	0.00	0.17			0.46	0.00	0.04		0.66		0.4		
B13	0.14					0.01			0.05	0.13	0.51	0.58	0.01			0.00	0.15				0.00	0.04		0.01		0.5	0.7	

Chemical composition (volume concentration, in 10^{17} cm^{-3} units) and H content (in at.-%; H-b, H-u, H-a stand for H concentrations in bound, unbound, and bound after annealing states, respectively) of HTG and MG ZnO crystals. `0.00' means that the corresponding element was detected, but rounding gives zero concentration within the given precision; underlined numbers specify upper limits.



G. Brauer, J. Kuriplach
Hydrogen in ZnO – a challenge to experiments and theory
72. Jahrestagung der DPG und DPG Frühjahrstagung des Arbeitskreises Festkörperphysik
Berlin, 25.-29.02.2008

Scattering of the c-lattice constant of different ZnO crystals with respect to a reference value from the literature. MT stands for an MT-06 sample.

Positron lifetimes in ZnO (more systematic studies)

high precision positron lifetime measurements at Prague

Summary of all systematic experimental results

Positron lifetimes:	ALL crystals investigated show SATURATION TRAPPING
	HT crystals: 180-182 ps; MG crystals: 165-167 ps
Impurities:	vary among suppliers and year of crystal growth; always (much) below 10 ppm
Saturation trapping:	requires more than 100 ppm
H content:	unbound: not every specimen; chemically bound: much higher than 1,000 ppm
Microstructure:	mosaic structure and internal stress depend on supplier; only IKZ samples show macroscopic crystallites with almost no stress

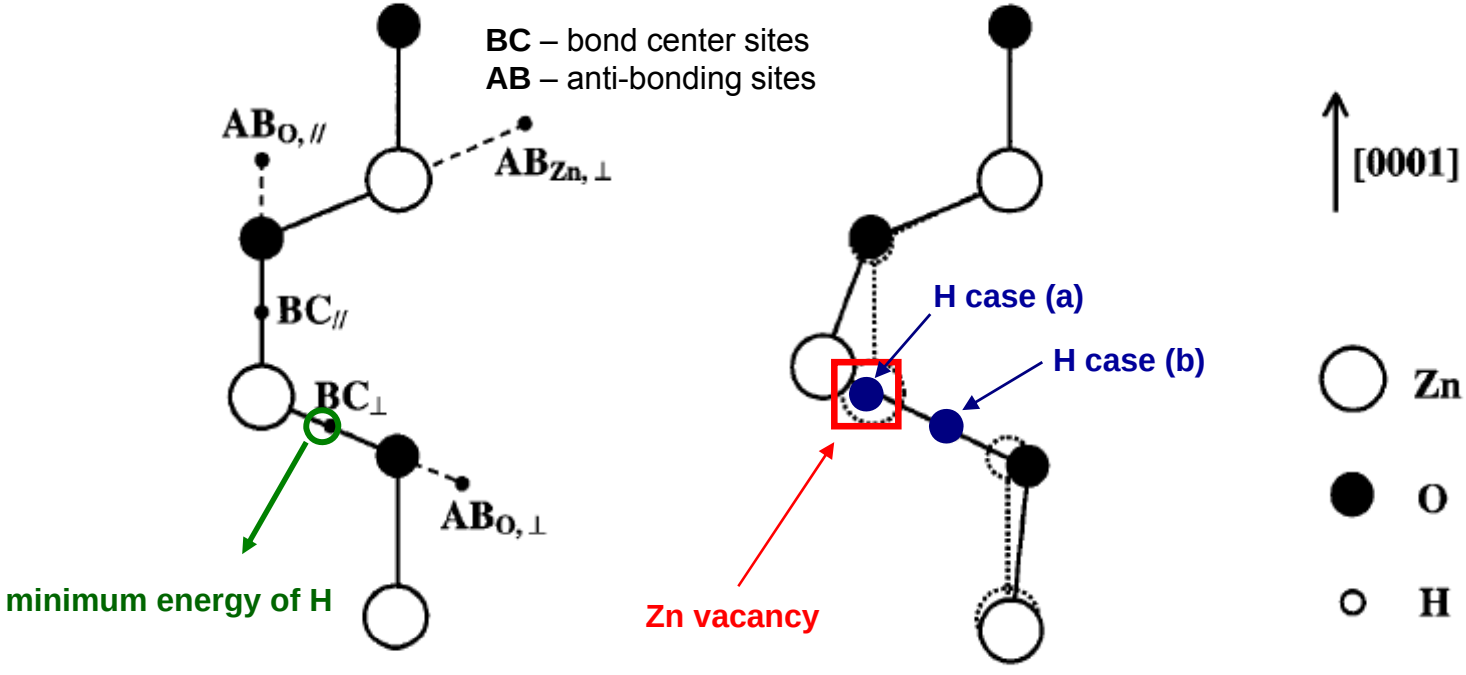
Conclusions:

Defects seen by positrons depend on the growth method of crystals

Two types of open volume defects being smaller than V_{Zn} due to chemically bound H exist

Positron lifetimes in ZnO (more theoretical calculations)

rigid lattice:(0001) plane relaxed lattice:(0001) plane



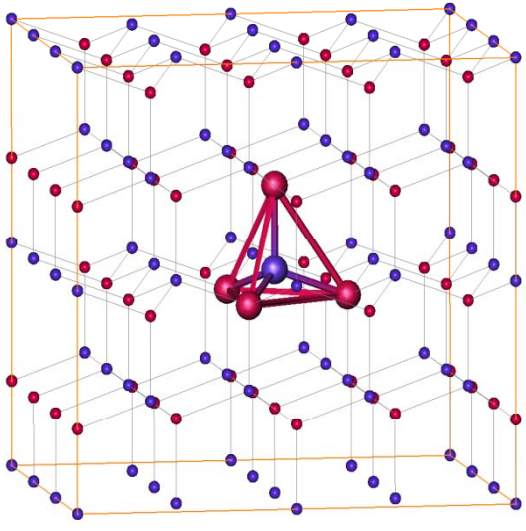
Ch. G. Van de Walle, Phys. Rev . Lett. 85, 1012 (2000)

Very first and still rough calculations (relaxed lattice) by ATSUP:

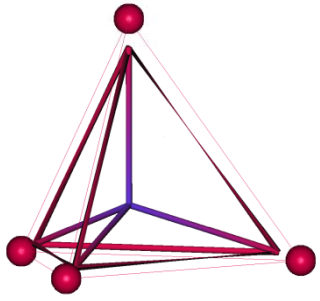
G. Brauer, J. Kuriplach, J. Cizek, W. Anwand, O. Melikhova, I. Prochazka, W. Skorupa, Positron lifetimes in ZnO single crystals, Vacuum 81 (2007) 1314-1317

- case (a) - H directly in the center of Zn vacancy (maximum shortening): τ = **185 ps**
- case (b) - H position $BC_{\perp}$ unchanged by formation of vacancy (smaller shortening): τ = **207 ps**

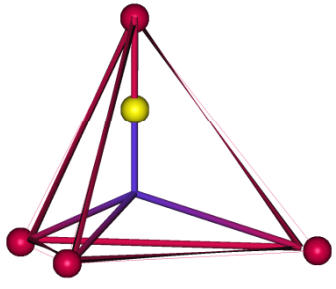
Positron lifetimes in ZnO (more theoretical calculations)



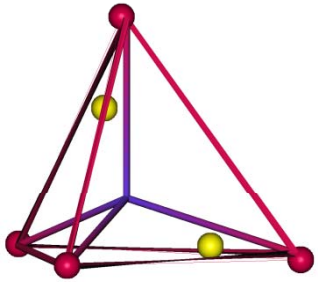
(a)



(b)



(c)



(d)

(a) ZnO perfect lattice (hexagonal, Wurtzite) together with the identified ZnO_4 'structure building unit' (red/blue tetrahedron)

Examples of atomic configurations of studied defects: (b) V_{Zn} (c) V_{Zn}+1H (d) V_{Zn}+2H

The size of relaxations of Zn and O atoms can be seen from the deviation of spheres representing atoms from ideal positions represented by the corners of tetrahedra. Distances between H and neighboring O atoms are ~1 Å.

Positron lifetimes in ZnO (more theoretical calculations)

Configurations of selected H-related defects from VASP code by relaxing the total energy with respect to atomic positions

Results: H inside V_O is located in the vacancy center
H inside V_{Zn} are located in the so-called bond-center positions
H_2 molecule is not stable inside V_{Zn}

VASP relaxed supercells were extended by adding the perfect ZnO lattice at sides to minimize the effect of boundary conditions on positron characteristics

Self-consistent electron density and potential were used for positron calculations to account for the charge transfer between Zn and O atoms (i.e. ionicity of Zn-O bonds)

Positron lifetime calculations finally by ATSUP (with BN enhancement factor)

Results

MG crystals (165-167 ps) almost correspond to V_{Zn}+2H complexes

HTG crystals (180-182 ps) could better correspond to V_{Zn}+1H complexes

calculated τ_b (154 ps) in good agreement with experiment (151 $\pm$ 2 ps)

models/discussion in literature consider so far only H_i, V_{Zn}+2H, and more recently H_O , i.e. definitely not the whole spectrum of possible H-related defects

Defect	Lifetime (ps)	Energy (eV)	Defect	Lifetime (ps)	Energy (eV)
bulk	154	—	V_{Zn}+1H	203	0.51
V_O	—	—	V_{Zn}+2H (||)	164	0.03
V_O+1H	—	—	V_{Zn}+2H	164	0.03
V_{Zn}	246	1.25	V_{Zn}+3H (||)	—	—
V_{Zn}+1H (||)	199	0.48	V_{Zn}+3H	—	—

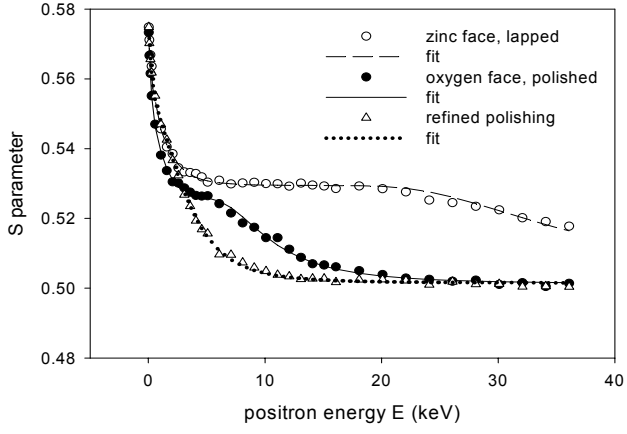
Further improvements in the present calculations are in progress:
taking into account positron induced forces
consideration of charge states

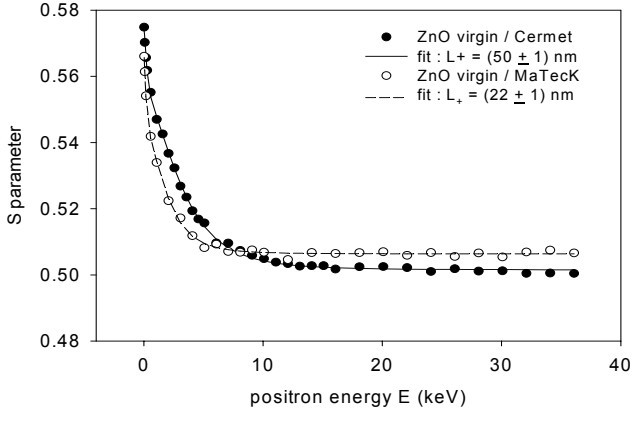
SPIS results on ZnO single crystals

Judgement of crystal quality

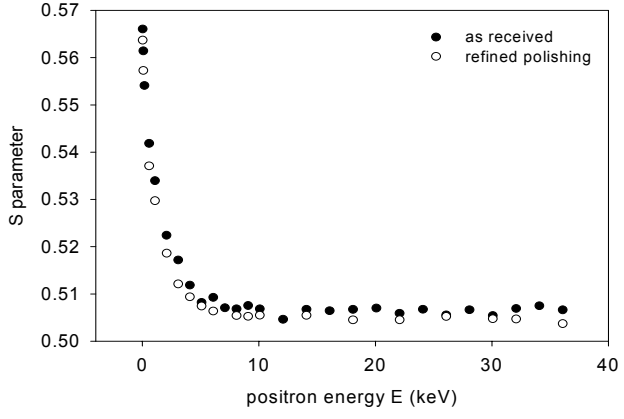
Problem: - no defect-free ZnO reference exists yet for comparison !!!

MG (Cermet 2002)





HTG (MaTecK 2004)



MG: # damaged sub-surface layer introduced by lapping (Zn face, d = (1,942 ± 32) nm) and polishing (O face, d = (231 ± 5) nm)

refined polishing can remove this damage and gives L_+ = (50 ± 1) nm

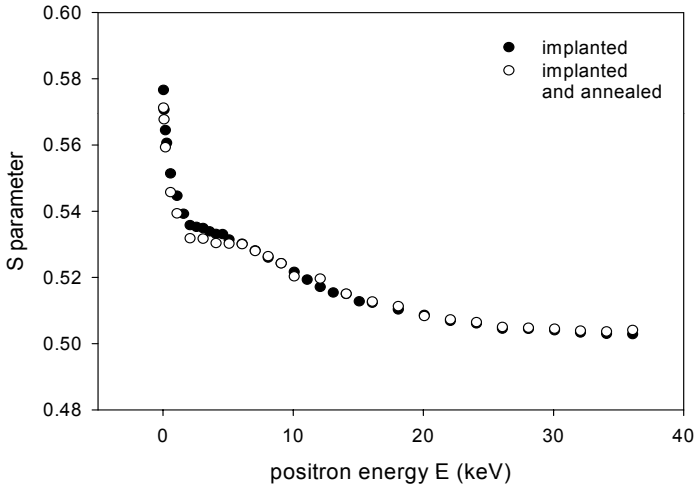
HTG: # no sub-surface damage detected

marginal improvement of surface quality by refined polishing gives L_+ = (22 ± 1) nm

G. Brauer, W. Anwand, W. Skorupa, J. Kuriplach, O. Melikhova, J. Cizek, I. Prochazka, C. Moisson, H. von Wenckstern, H. Schmidt, M. Lorenz, M. Grundmann
Comparative characterization of differently grown ZnO single crystals by positron annihilation and Hall effect
Superlattices and Microstructures 42 (2007) 259-264

SPIS results on ion implanted ZnO single crystals

MG, Cermet 2002



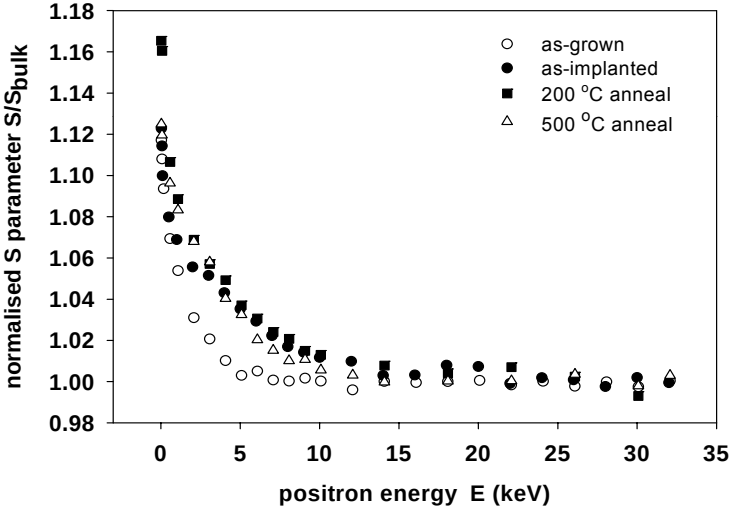
150 keV N^+, 1 x 10^{14} cm^{-2}, at 300 °C
(perpendicular to the sample surface)

annealing: 500 °C, 30 min, air

damaged layer: *d* = (354 ± 7) nm

TRIM: expected damage profiles
~200 nm (peak of vacancies profile)
~270 nm (peak of ions profile)

HTG, MaTecK 2004



40 keV N^+, 1 x 10^{15} cm^{-2}, at RT
(sample 7° tilted to surface normal)

annealing: 200 °C, 500 °C, 30 min, oxygen

no box-shaped or Gaussian profile could be fitted !

damaged layer: 10 nm < *d* < 170 nm

TRIM: ~42 nm (vacancies) ; ~ 72 nm (ions)

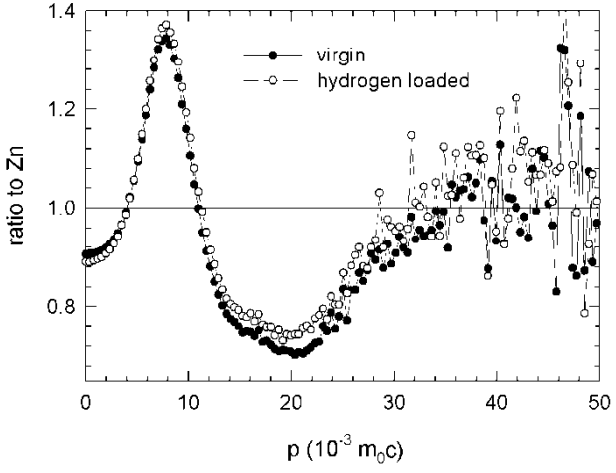
Conclusions:

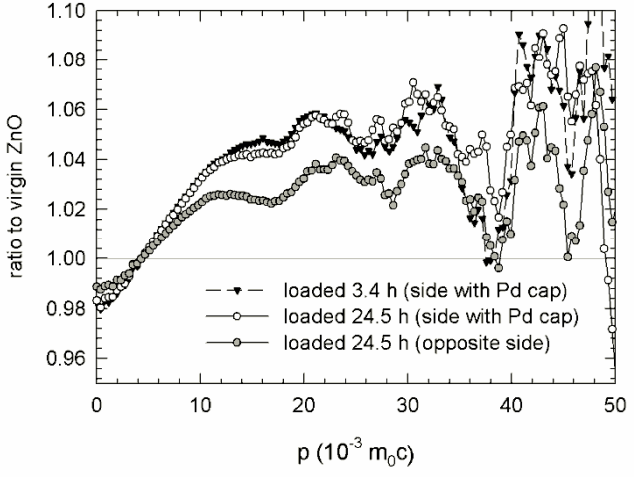
damage created by ion implantation can generally be detected by SPIS
width of damaged layer can be estimated

ZnO electrochemically doped with hydrogen (positron lifetime, CDB)

J. Cizek, N. Zaludova, M. Vlach, S. Danis, J. Kuriplach, I. Prochazka, G. Brauer, W. Anwand, D. Grambole, W. Skorupa, R. Gemma, R. Kirchheim, A. Pundt
Defect studies of ZnO single crystals electrochemically doped with hydrogen
J. Appl. Phys. 103 (2008) 053508 (8 pp)

Virgin sample contains 0.3 at.-% H (chemically bound) and less than 0.1 at.-% unbound H
H loading up to ~ 30 at.-% achieved - more than half of this amount is chemically bound !
marginal drop of τ from 182 ps to 179 ps due to H loading



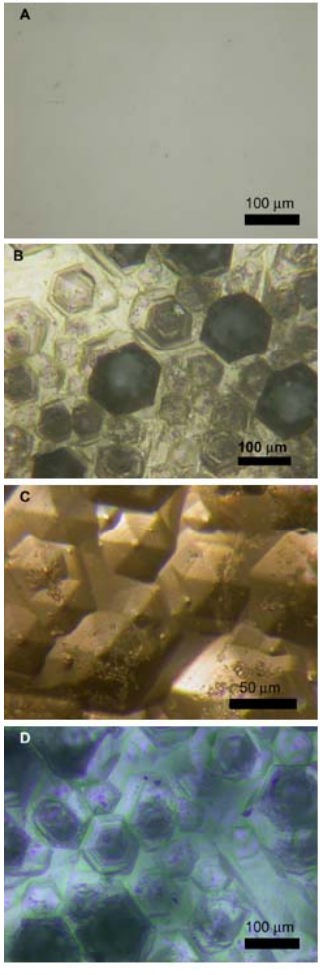


CDB ratio curves related to pure well annealed Zn

Due to trapping at V_{Zn} , positrons are sensitive only to H bound in the vicinity of V_{Zn}
H loading causes increase at $p \sim (8 \times 10^{-3})\ m_0c$, shallower minimum at $p \sim (20 \times 10^{-3})\ m_0c$
This increase is caused by annihilations with electrons belonging to O-H bonds

CDB ratio curves related to a virgin ZnO crystal

These curves show exclusively the effect of H loading
Obviously a broad peak is caused at the high momentum range (5 - 38) × 10-3 m_0c



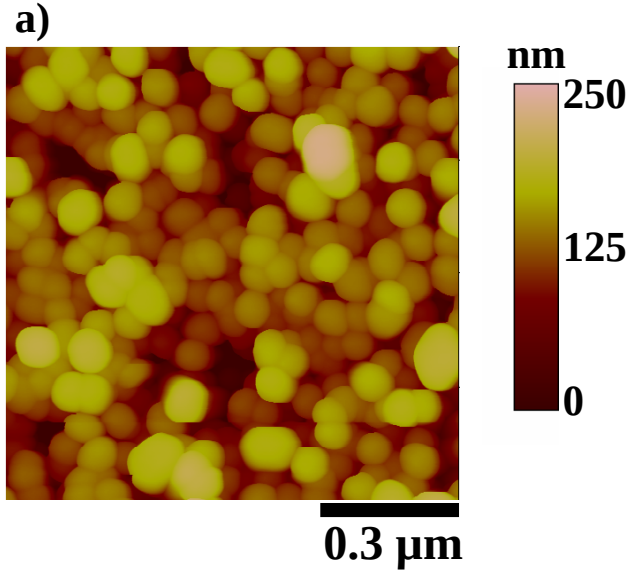
Optical Microscopy images of the ZnO crystal surface before (A) and after (B thru D) 24.5 h H loading:
(B) reflected light, (C) cross light,
(D) UV light (in transmission)

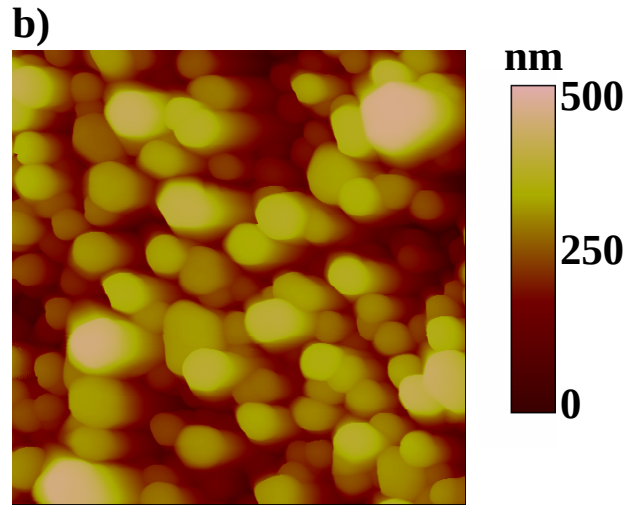
Investigation of ZnO nanorods (AFM, SPIS)

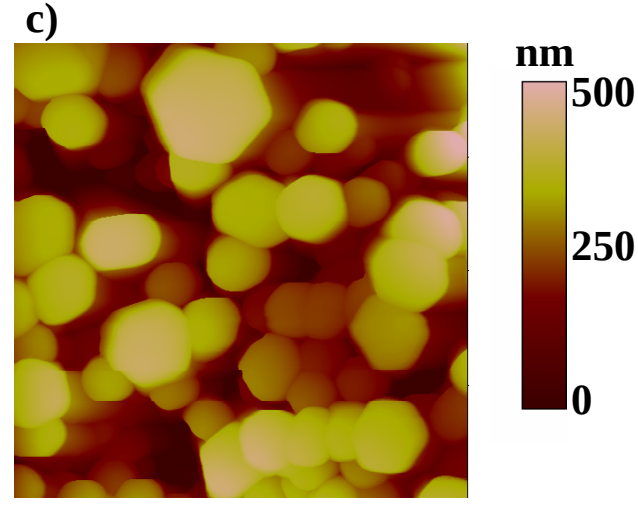
GOAL: fabrication of solar cells for inexpensive solar energy conversion (blend of a light-absorbing, hole conducting polymer and a grown array of high-quality vertical ZnO nanorods)

preparation technology of ZnO nanorods
- # Si (100) used as a substrate
- # ZnO seed layer converted from Zn acetate;
- # details: L.E. Greene, et al., Nanoletters **5** (2005) 1231

different rod lengths' available from U Hong Kong:
(a) ~200 nm, (b) ~350 nm, (c) ~500 nm



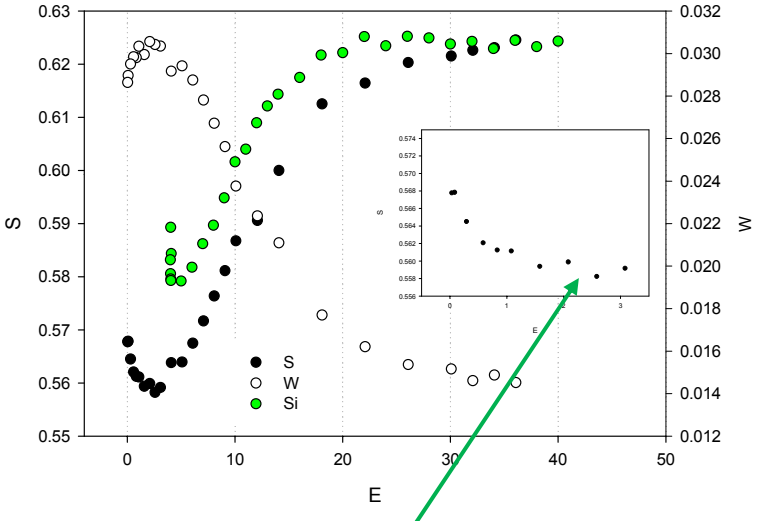




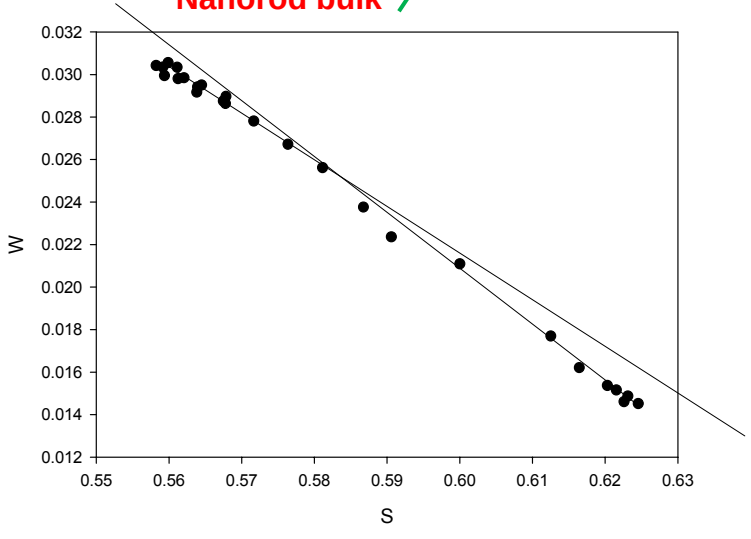
G. Brauer, W. Anwand, D. Grambole, W. Skorupa, Y. Hou, A. Andreev, C. Teichert, K. H. Tam, A. B. Djurisic
Non-destructive characterization of vertical ZnO nanowire arrays by slow positron implantation spectroscopy, atomic force microscopy, and nuclear reaction analysis
Nanotechnology 18 (2007) 195301 (8 pp)

Investigation of ZnO nanorods (AFM, SPIS)

SPIS



Nanorod bulk



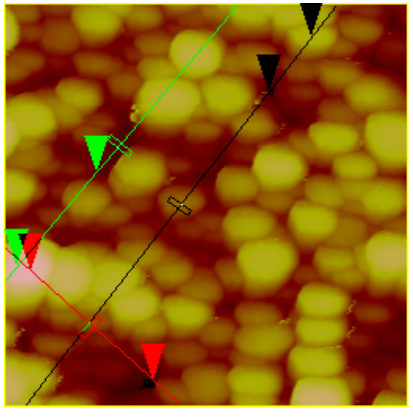
~200 nm rod length (expected from preparation condition) studied

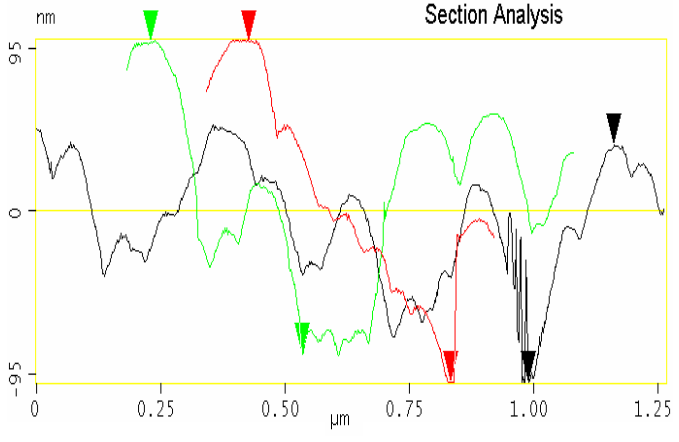
S(E) for Si(100) with natural SiO_2 layer for comparison (green curve)

ZnO single crystal (MG, Cermet 2002) bulk = reference (Sref = 0.5013)

jump in S at 3-4 keV should be due to influence of SiO_2
- # only positrons up to ~3 keV annihilate in ZnO nanorods
- # influence visible also in S-W plot (no straight line !)

evaluation results and conclusions for ZnO:
- # ZnO nanorods grown on a ZnO layer of ~80 nm thickness
- # ~10 % increase in S means large vacancy-type defects
- # L_+ = (1.5 ± 0.5) nm estimated





AFM standard Si tip (tapping mode)
area of a selected rod: ~10761 nm², diameter: ~117 nm
heights of the rods: ~130 nm to ~210 nm
(match to predicted height of ~200 nm from preparation)

Investigation of ZnO nanorods (AFM, SPIS, PL, SEM)

preparation technology of ZnO nanorods at U Hong Kong:

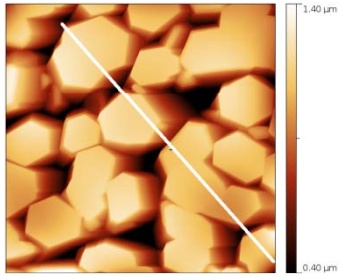
Si (100) used as a substrate
thermal evaporation (TE), ~ 1.2 μm length
hydrothermal growth (HT), ~ 1.2 μm length

PL and SEM at HKU
AFM / C-AFM at Montanuniversität Leoben / Austria
SPIS at FZD

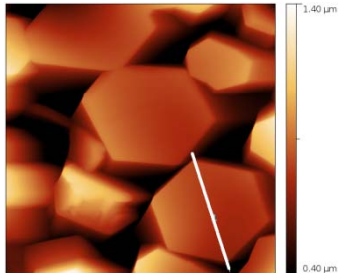
C. Teichert, Y. Hou, A. Andreev, G. Brauer, K.H. Tam, A. Djurisic
Characterization of vertical arrays of ZnO nanorods by AFM
Materials Research Society (MRS), 2007 Fall Meeting ,
Boston/MA, 26.-30.11.2007

(TE)

5 μm

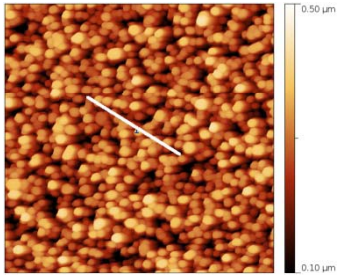


2.5 μm

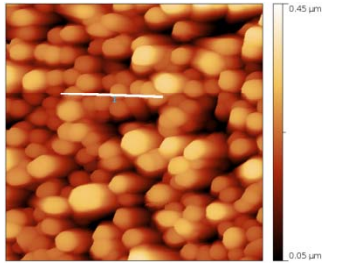


(HT)

2.5 μm



1 μm



Common presentations at PPC-9 conference, Wuhan / P.R. China, May 11-15, 2008

G. Brauer, W. Anwand, W. Skorupa, I. Beynik, C. Teichert, Y.F. Hsu, Y.Y. Xi, C.Y. Zhu, C.C. Ling, and A.B. Djurisic
("Experimental results on ZnO nanorods")

J. Kuriplach, G. Brauer, O. Melikhova, J. Cizek, I. Prochazka, W. Anwand, W. Skorupa
Vacancy – Hydrogen Complexes in ZnO (theory)

Investigation of thin ZnO films

magnetron-sputtered ZnO on indium-tin oxide (ITO) coated glass

covered by Al_2O_3 layer ; aluminum contacts

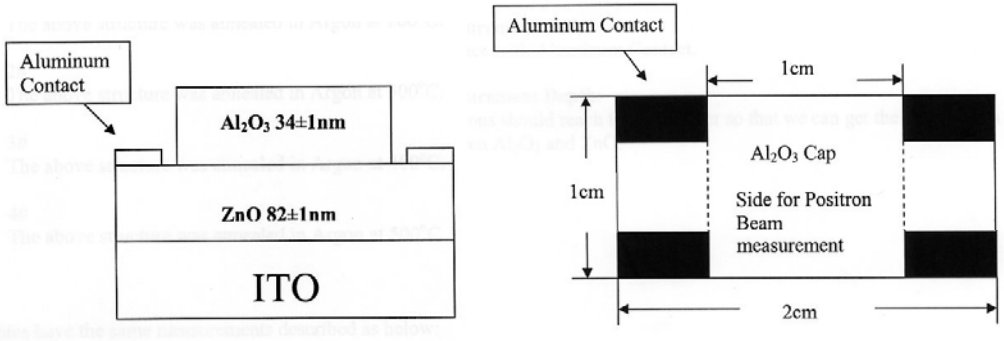
investigations by PL, DLTS, and SIMS : results strongly connected

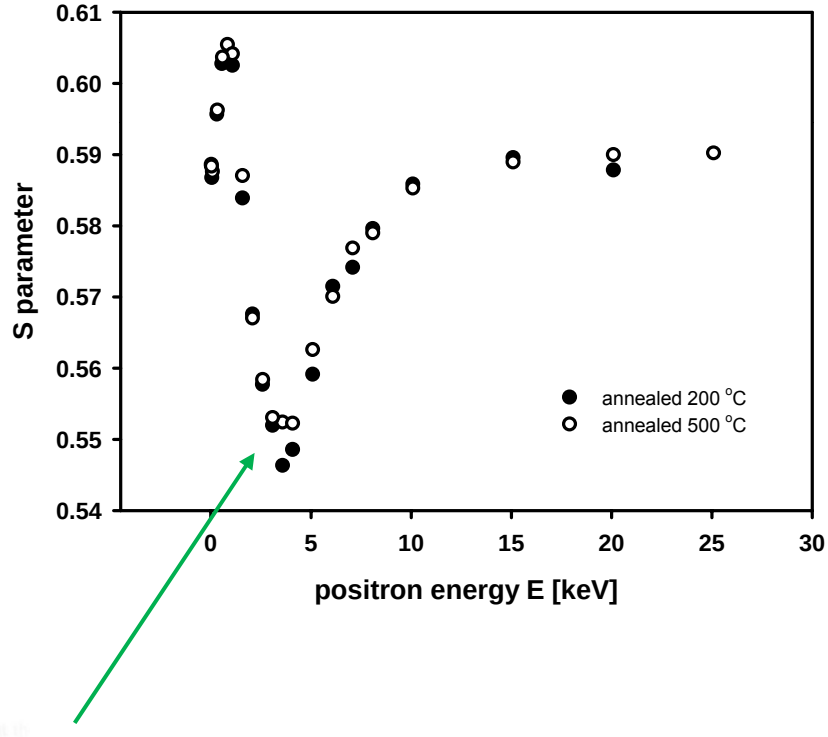
Zn outdiffuses from ZnO to the oxide layer during annealing

deep level defects near the interfacial region created, which reduce the band-edge emission and increase the deep level emission at 2.37 eV

optical and electrical properties disturbed

Studies of oxide/ZnO near-interfacial defects by photoluminescence and deep level transient spectroscopy
R.S. Wang, Q.L. Gu, C.C. Ling, H. C. Ong
Appl. Phys. Lett. 92 (2008) 042105





 # vacancy-type defects clearly visible in our laboratory positron beam „SPONSOR“

 # CDB possible at our laboratory beam „SPONSOR“ (stronger positron source highly needed)

 # specimens for first EPOS measurements ???

 # nature of these defects ???

 # can SPIS help to identify ???

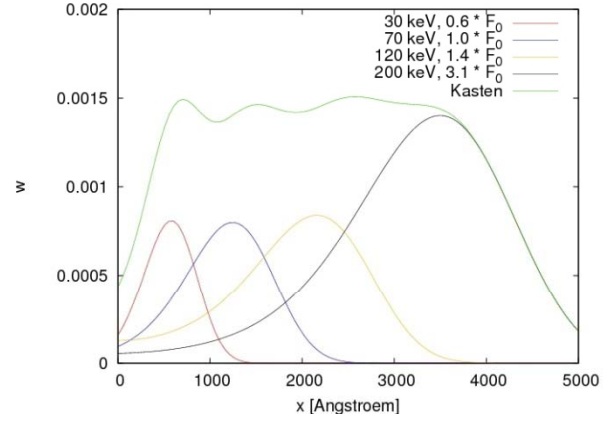
Doktorand Matthias Schmidt (FZD / U Leipzig : 2007-2009)
Promotionsthema : “p-Dotierung von ZnO durch Ionenimplantation”

Ionenimplantation (FZD)
elektrische und optische Charakterisierung (U Leipzig)
SPIS (FZD)
PLEPS (FRM-II Garching):

Proposal eingereicht	(Januar 2008)
Proposal akzeptiert	(März 2008)
Zuteilung 2 Tage Messzeit	(Mai / Juni 2008)

Wiederholung aller Messungen nach thermischer Ausheilung der Proben (500 °C, 30 min, an Luft)

SRIM calculations



Homo-epitaktische ZnO-Dünnfilme (ZnO-Substrat, Einkristall)

Tiefenabhängigkeit der Positronenlebensdauer (0.5 – 20 keV) an einer virgin-Probe
Positronenlebensdauermessung in einer ionenimplantierten Schicht (7,5 keV) für drei verschiedene Fluenzen (= 3 Proben)

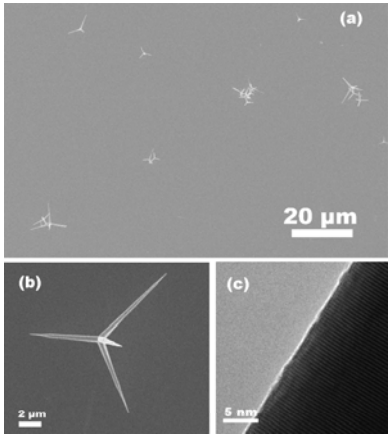
Hetero-epitaktische ZnO-Dünnfilme (Saphir-Substrat, Einkristall)

Tiefenabhängigkeit der Positronenlebensdauer (0.5 – 20 keV) an einer virgin-Probe
Positronenlebensdauermessung in einer ionenimplantierten Schicht (7,5 keV) für drei verschiedene Fluenzen (= 3 Proben)

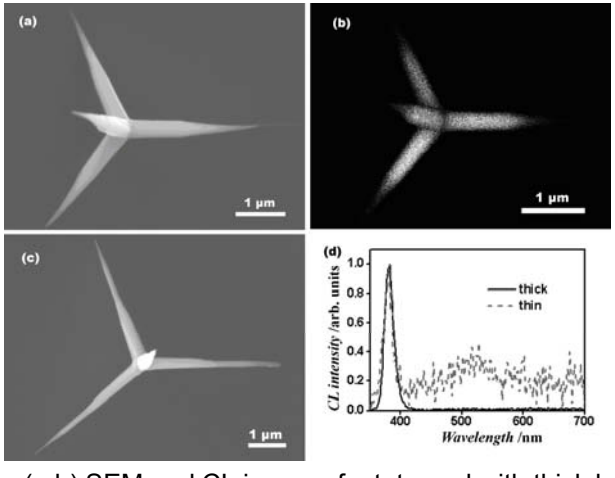
Hetero-epitaktische ZnO-Dünnfilme (Saphir-Substrat, 2“-wafer)

Tiefenabhängigkeit der Positronenlebensdauer (0.5 – 20 keV) an einer virgin-Probe
Positronenlebensdauermessung in einer ionenimplantierten Schicht (7,5 keV) für drei verschiedene Fluenzen (= 3 Proben)

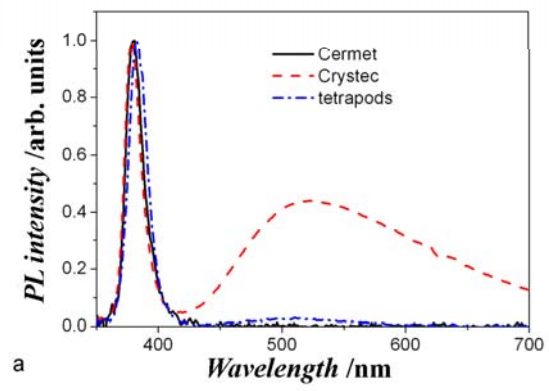
Investigations on ZnO tetrapods (PL, time- resolved PL, ICP-MS)

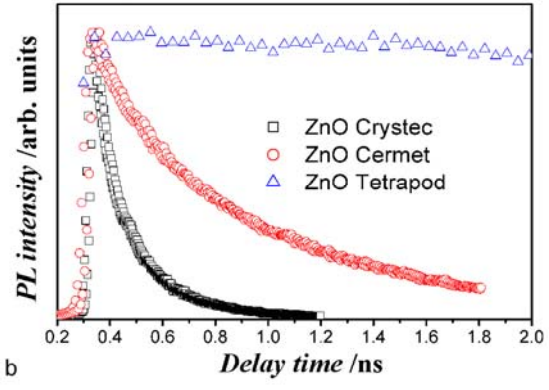


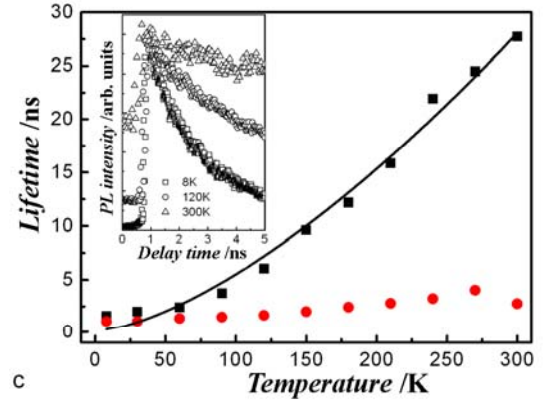
(a), (b) SEM images of dispersed tetrapods on Si and an individual tetrapod
(c) Representative HRTEM image of an individual tetrapod leg



(a,b) SEM and CL image of a tetrapod with thick legs
(c) SEM image of a tetrapod with thin legs
(d) Comparison of CL spectra of the tetrapods with thick and thin legs







(a) PL spectra of the tetrapods and single crystals
(b) Time resolved PL decay curves
(c) Temperature dependence of decay constants in tetrapods

squares = tetrapod without defect emission
solid line = least-squares fit using $\alpha+\beta T^{3/2}$
circles = tetrapods with defect emission.

High quality ZnO epilayers needed for fabrication of light emitting diodes

Device performance strongly relies on improvements in materials quality (presence/ activity of defects)

Nanostructures are so far expected to be more defected than single crystals or thin films / epilayers

PL and time-resolved PL are used to judge the materials quality (exciton lifetime)

Identification of defect structures is needed to understand/improve the materials of technological importance

Common paper is in progress for **ADVANCED FUNCTIONAL MATERIALS**

Acknowledgements / Cooperations (ZnO)

Special thanks to my colleagues at:

FZD:	W. Anwand D. Grambole H. Schmidt W. Skorupa
Charles U Prague:	J. Cizek J. Kuriplach O. Melikhova I. Prochazka
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Hong Kong U:	C.C. Ling A.B. Djurisic
Montan-U Leoben:	C. Teichert
U Göttingen:	A. Pundt
U Bath:	P.G. Coleman

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DAAD D / 08 / 01769 (PPP mit Hong Kong, 2008 / 2009)

Using positron annihilation for research is like climbing a mountain on a seldom route – you will savour the moment when you are the first at the top !