2nd/March/2000/Erlangen

Investigation of SiC by Positrons

Atsuo KAWASUSO

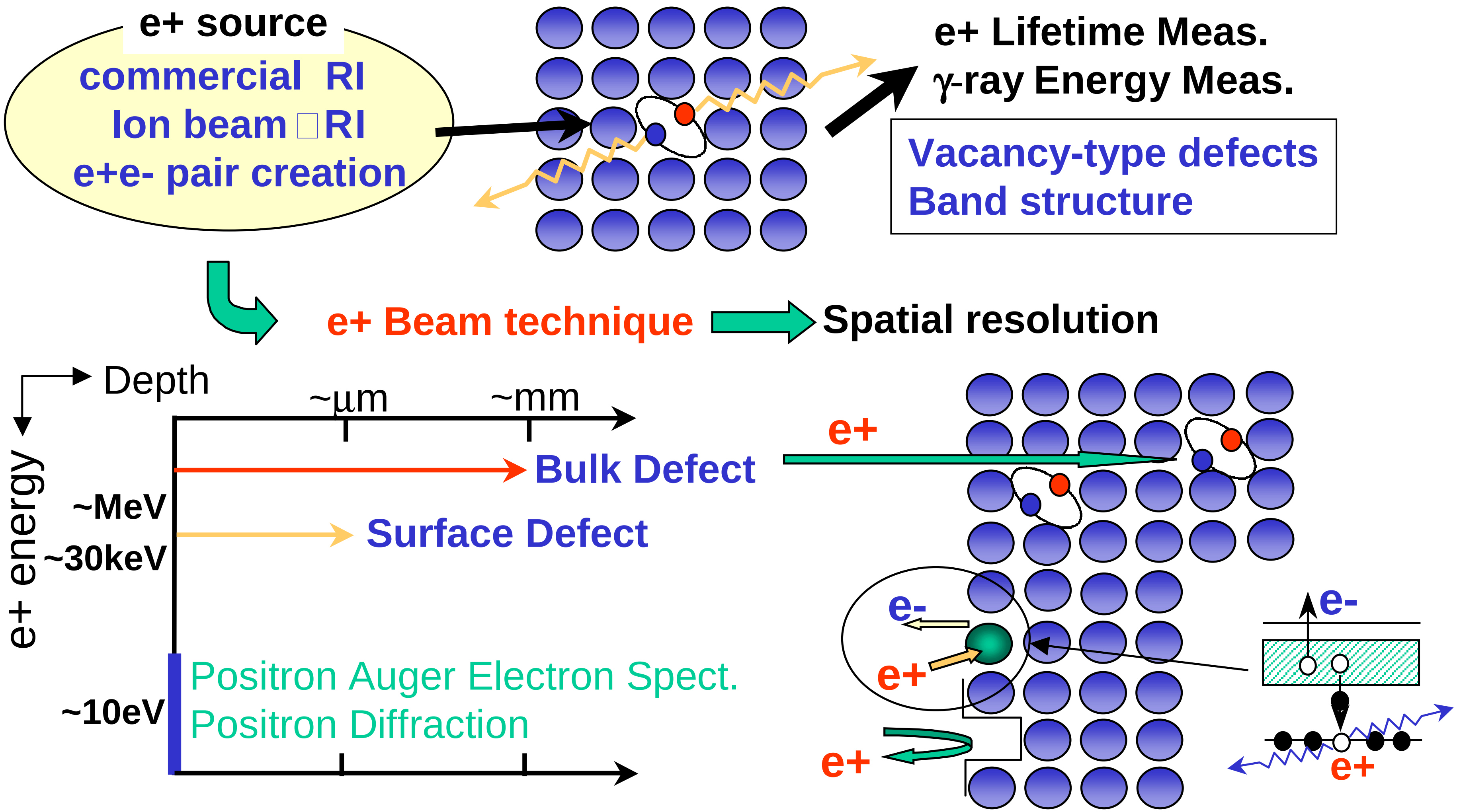
Martin-Luther-Universität Halle-Wittenberg
(Humboldt Research Fellow)

Japan Atomic Energy Research Institute
Takasaki Establishment

contents:

- **Positron Study of Solid Materials**
- **Defects in SiC induced by e^--irradiation**

Positron (e+) Study of Solid Materials



e+ spectroscopy
Other methods

combination →

Probable characterization of defects in materials

1. Defects in SiC

<u>Fundamental defects</u>

Extended defects (dislocation, micro- and nano-pipes…)

Surface and interface (oxide, metallic overlayers….)

Impurities

<u>Point defects (vacancies, interstitials, anti-site, complexes)</u>

Functional

Carrier lifetime control

Impurity diffusion

Harmful

Scattering and recombination centers for carriers

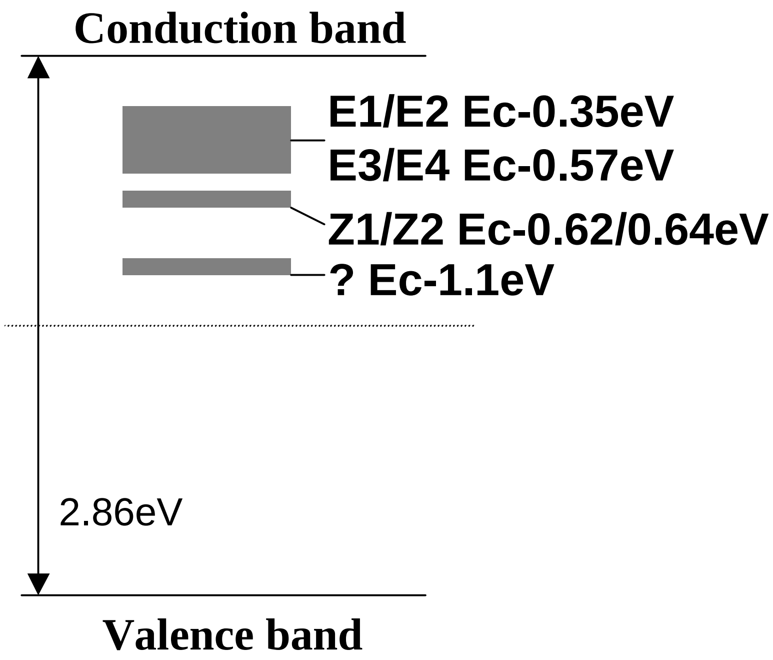
Establishment of Selective Doping by Ion Implantation

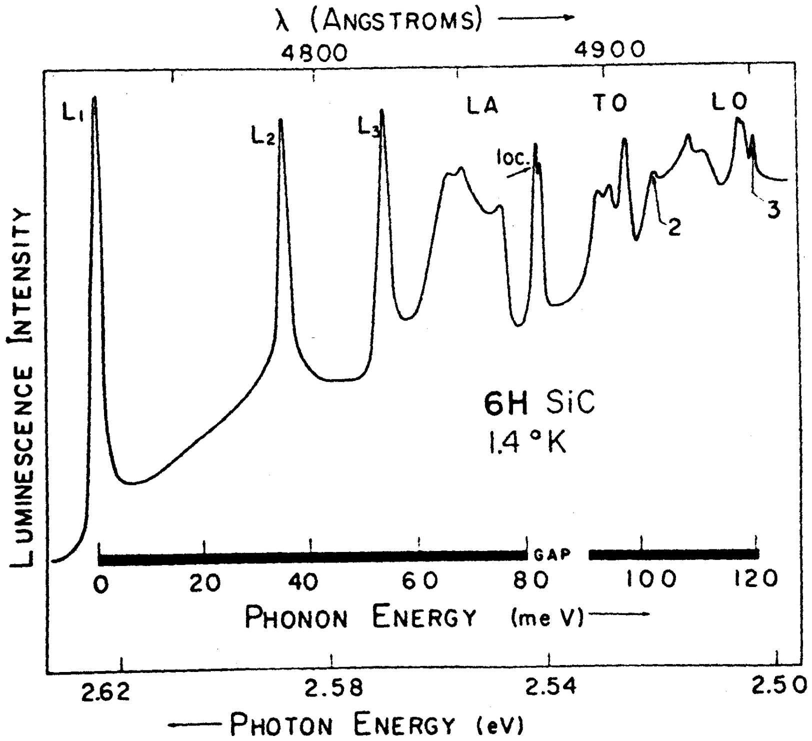
Control of Minority Carrier Lifetime

e-irradiation induced defects in SiC

DLTS studies (6H)
Zhang et al. (1989)
Ballandovich et al. (1986)

PL studies
Patrick&Choyke (1970~)





E1…E4….disappear at 1450^{o}C

Z1/Z2…remain even at 1700^{o}C

D1 lines…remain even at 1700^{o}C

Recent progress

6H SiC

D1 peaks — ▪ E1/E2 levels (***negative-U***)

4349A peak — ▪ Z1/Z2 levels (positive-U)

4H SiC

D1 peaks — ▪ Z1/Z2 levels (***negative-U***)

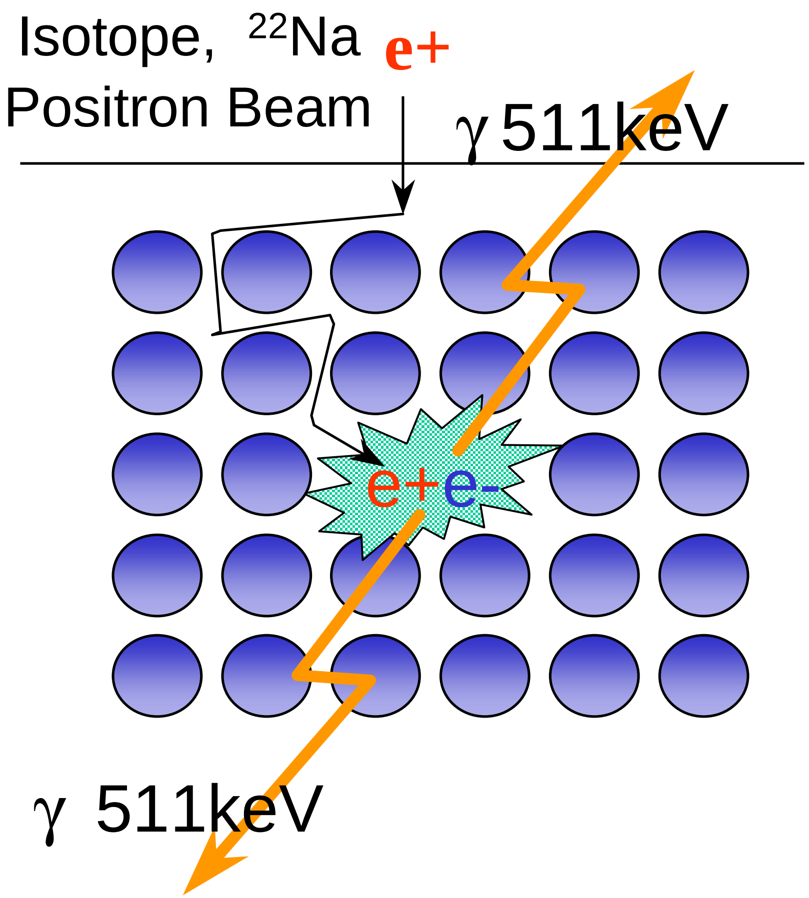
Hemmingsson et al. APL 74(1999)839, PRB 58(1998)R10199.

Frank et al. Proc. of ICSCRM'99.

⇩

Origin of Deep Levels ?

Positron Annihilation Spec. (PAS)



<u>e+ Lifetime</u>

$$\lambda = \tau^{-1} = \pi r_e c^2 \left| \int d^3 r \psi_+ \psi_- \right|^2$$

□ Vacancy Presence !
Vacancy Size

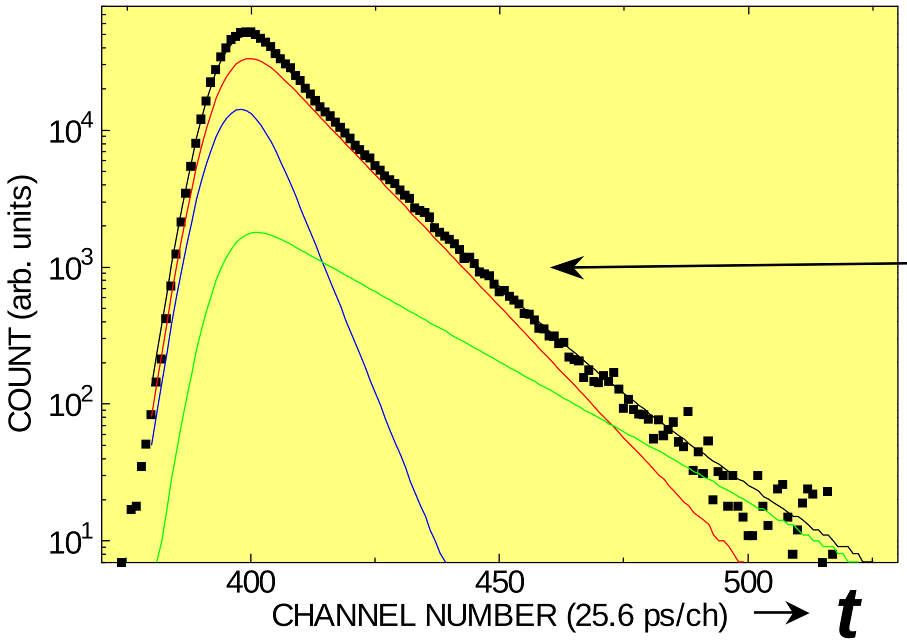
<u>Trapping Rate</u>

$$\kappa = \mu C_V$$

$$\mu = \frac{2\pi}{\hbar} \sum_{if} P_i \left| M_{if} \right|^2 \delta(E_i - E_f)$$

Doppler broadening measurement
- State of impurities bound at vacancies

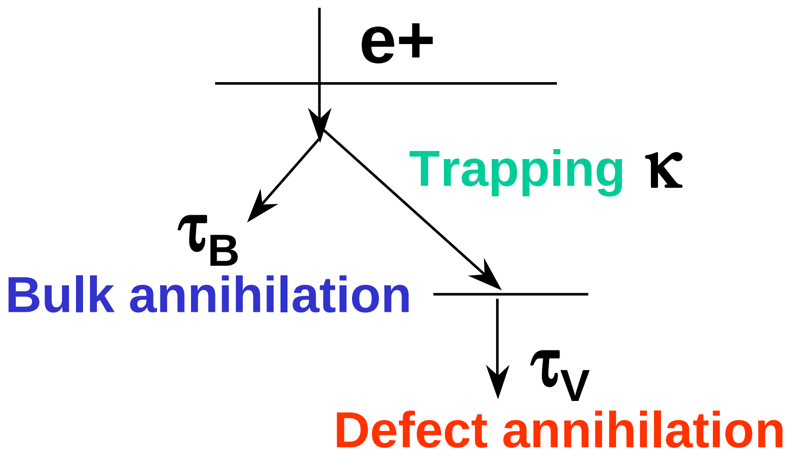
Analysis of Lifetime Spectrum



$$L(t) = \sum_{i=1}^{n} \frac{I_i}{\tau_i} \exp(-t / \tau_i)$$

$$\sum_{i=1}^{n} I_i = 100\%$$

Trapping Model



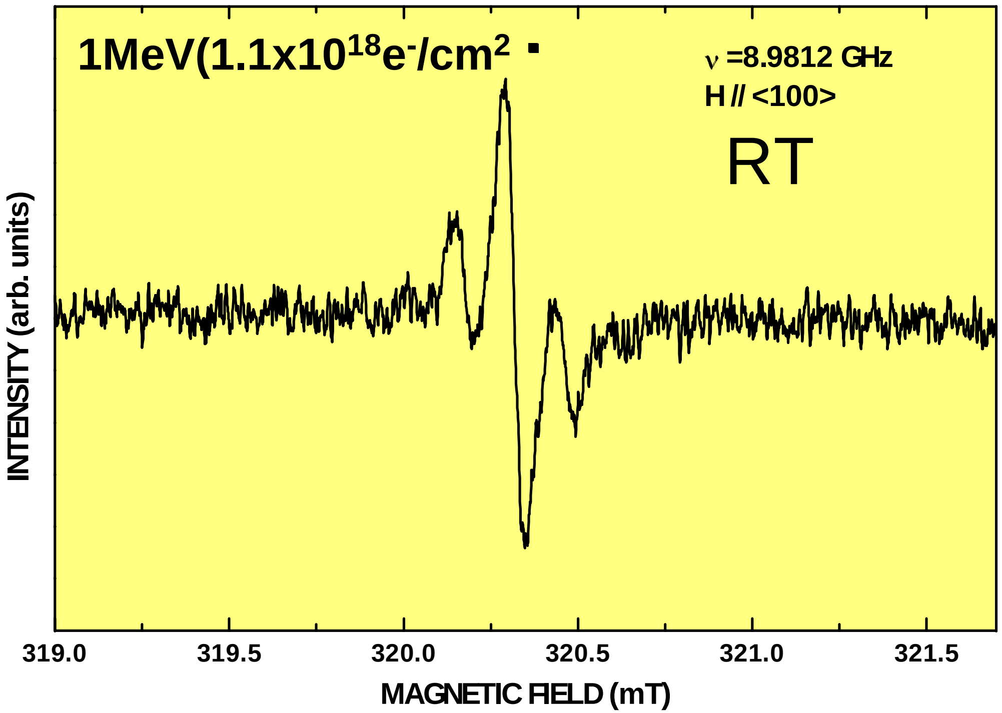
$$\tau_1 = \frac{1}{1/\tau_B + \kappa}$$

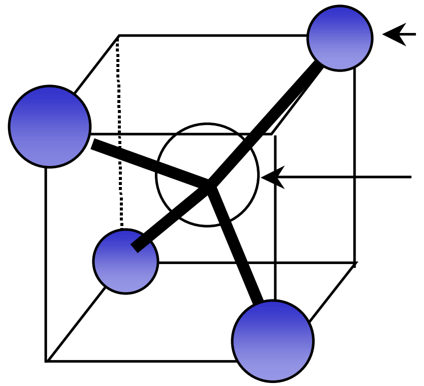
$$\tau_2 = \tau_V$$

$$\kappa = \frac{I_2}{I_1}(1/\tau_B - 1/\tau_V)$$

e-irradiated n-type 3C SiC

Kawasuso et al. AP A67(1998)209.





▪ =2.003, isotropic

▪ $_d$ symmetry → V_{Si}^{-}

Itoh et al. IEEE Trans.Nucl.Sci.37(1990)1732.

Balona and Loubser, J. Phys. C3(1970)2344.

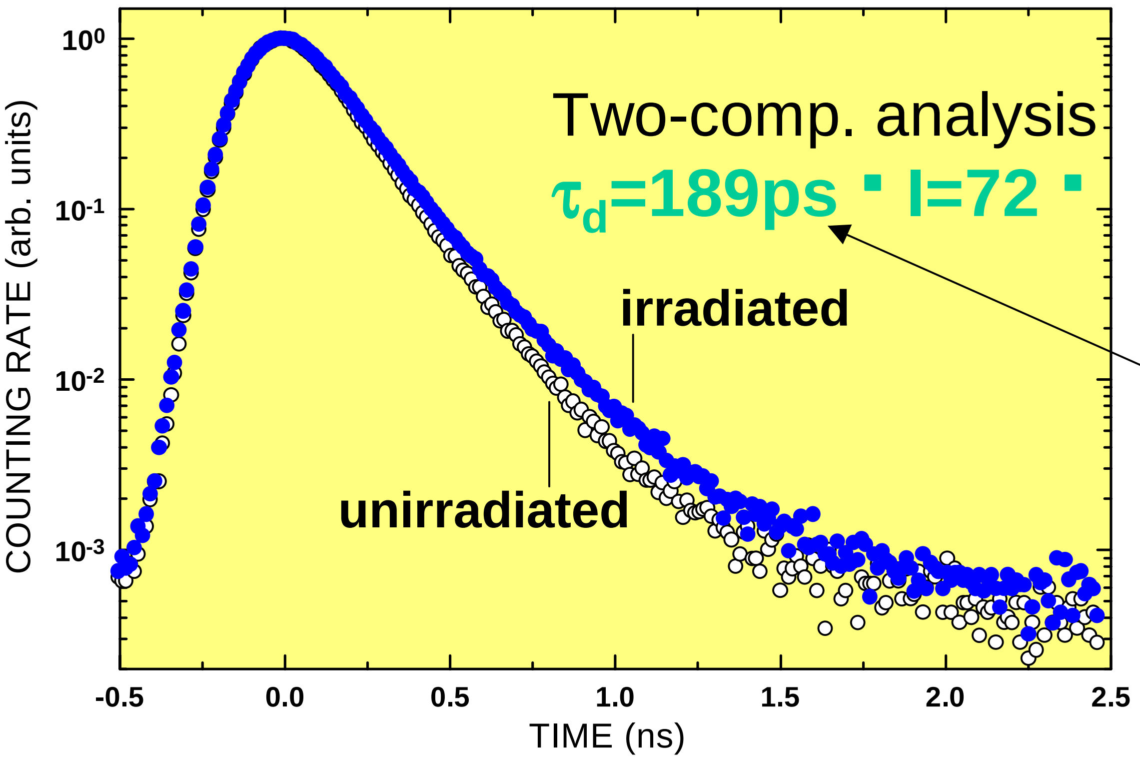
Table. Electron spin resonance parameters of centres produced in 3C and 6H SiC by electron and neutron irradiation

Spectrum	Model, S, temperature	g ($\pm 0{\cdot}0001$), D (cm^{-1})	$\lvert T \rvert \times 10^{-4}$ (cm^{-1}), Intensity	Annealing temperature, E (eV)
A 6H (−) (e, n)	V_C^0 $S = 1$ 77 K	$g = 2{\cdot}0020$ $D = 0{\cdot}0552$ $\phi = 44{\cdot}6°$ $\psi = 30°$	4·2 (1·5%)	200°C 1·25 eV
B 6H (±) (e, n)	V_C^- $S = \frac{1}{2}$ 300 K, 77 K	$g_\parallel = 2{\cdot}0032$ $g_\perp = 2{\cdot}0051$	2·8 (12%) 6·6 (6%)	1400°C 5·0 eV
[a]C 6H (−) (e)	$(V_C + V_C)^+$ $S = \frac{1}{2}$ 77 K	$g_\parallel = 2{\cdot}0050$ $g_\perp = 2{\cdot}0037$	3·8 (17%)	>1300°C >5 eV
D 6H (±) (e, n)	? $S = \frac{1}{2}$ 77 K	$g = 2{\cdot}0026$	—	>1300°C >5 eV
E 6H (±) (e, n)	V_C^+ $S = \frac{1}{2}$ >77 K	E1: $g = 2{\cdot}0034$ E2 $g_\parallel = 2{\cdot}0033$ $g_\perp = 2{\cdot}0028$	2·24 (10%) 4·48 (7%)	1400°C 5·0eV
F 3C, 6H (±) (e, n)	$(V_C + V_C)^-$ $S = \frac{1}{2}$ 300 K, 77 K	$g = 2{\cdot}0032$	2·62 (19%, 1·5%)	750°C 3·1 eV
G 6H (+) (n)	$(V_{Si} + B)^\circ$ $S = \frac{1}{2}$ 77 K	$g_\parallel = 2{\cdot}0001$ $g_\perp = 2{\cdot}0021$	$A = \pm 1{\cdot}04$ b $B = \mp 0{\cdot}3$	250 C 1·5 eV

a Visible only when the crystal is illuminated with infrared or visible light.

b These values refer only to the spectrum obtained when the magnetic field is rotated in a plane perpendicular to the hexagonal axis. The spectrum for other orientations has not been fully analysed.

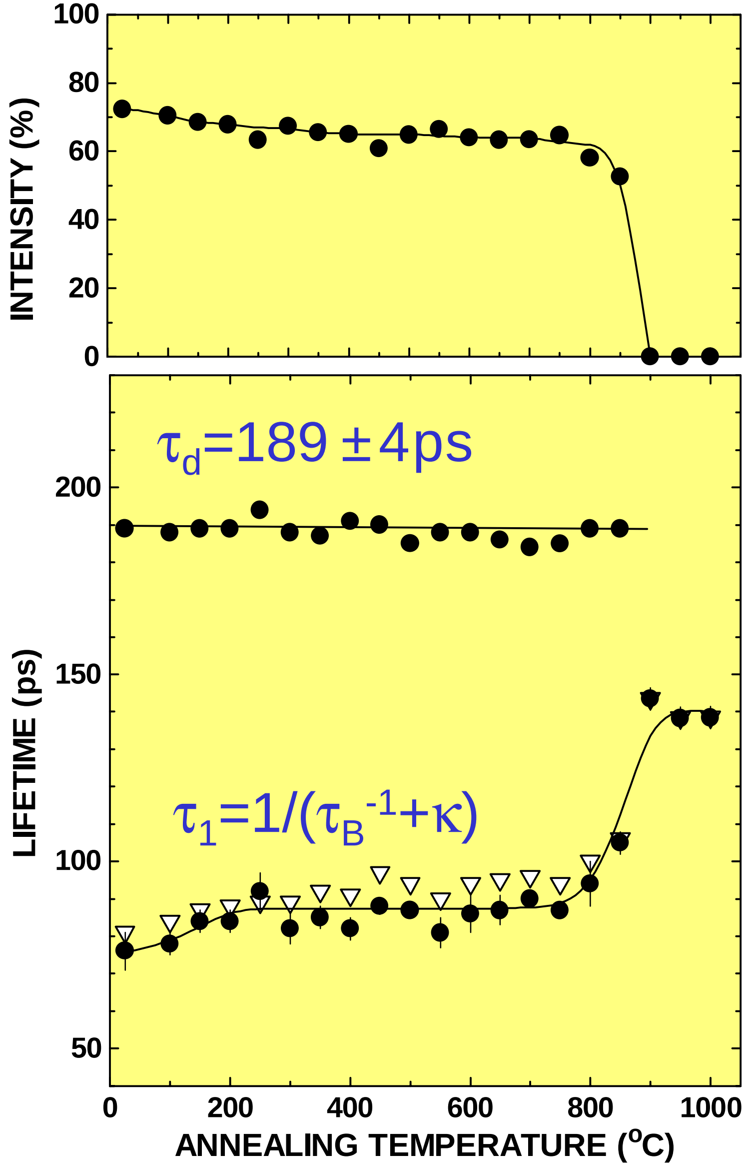
Positron Lifetime Spectrum

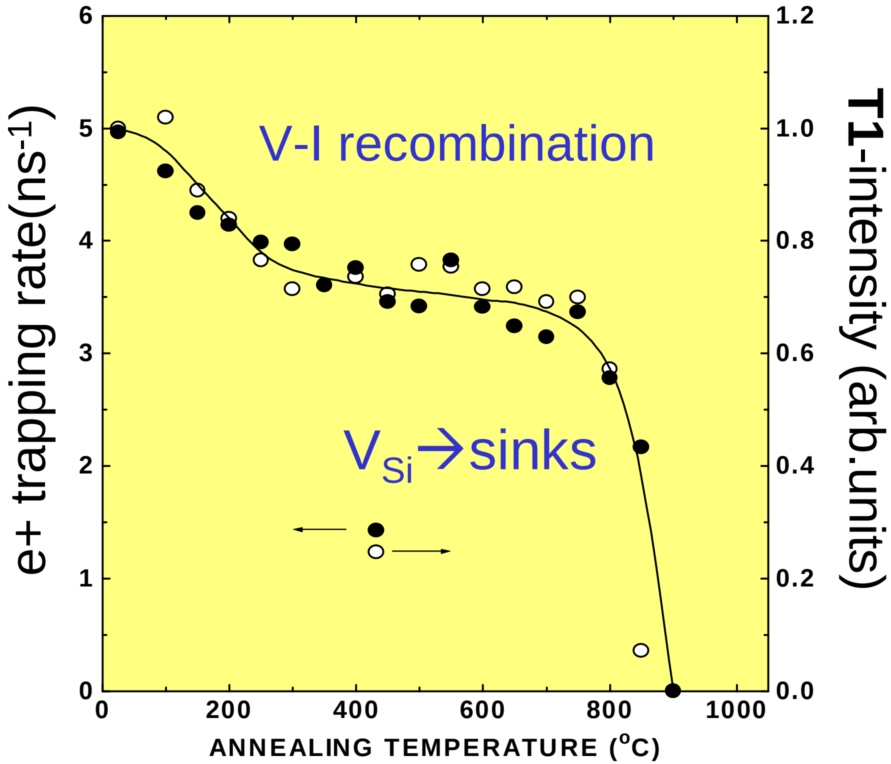


<u>Theoretical e+ lifetime</u> (Brauer et al)

Bulk	**…138ps**
V_C	**…153ps**
V_{Si}	**…191ps**
$V_{Si}V_C$	**…212ps**

Annealing of e+ lifetime and trapping rate



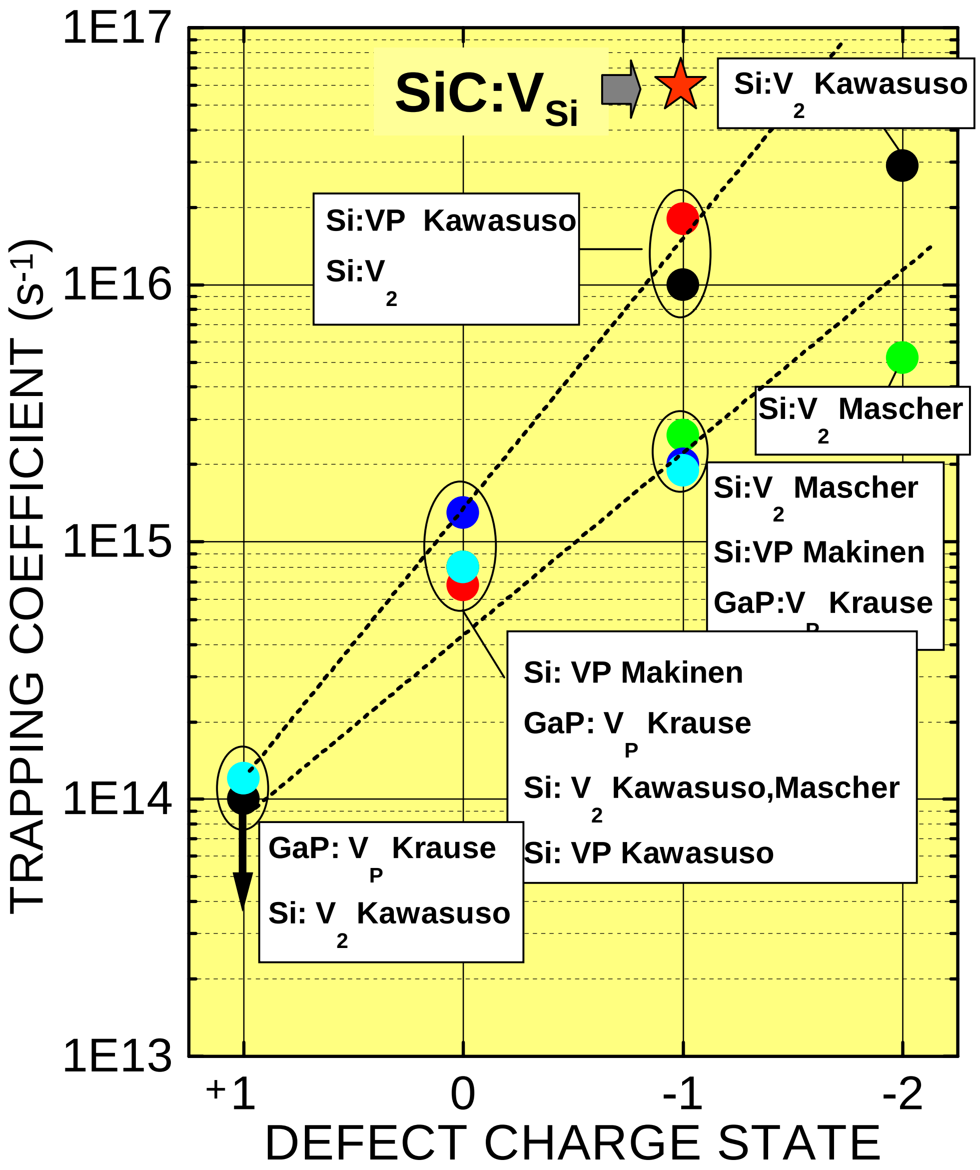


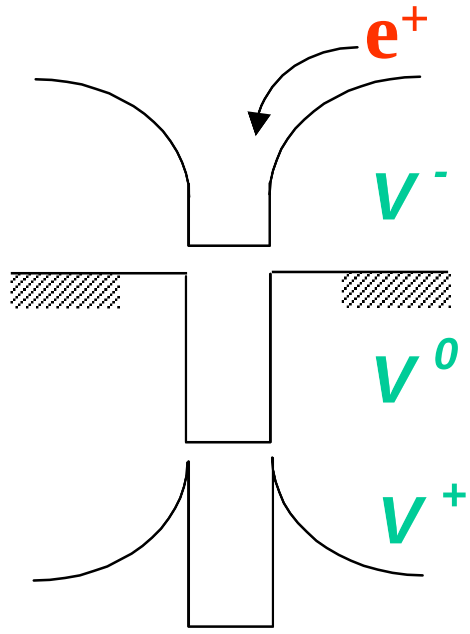
e+ trapping rate: $\kappa=\mu C_V$

μ~6x10^{16} s^{-1}

Determination of defect concentration

e+ trapping coefficient v.s. defect charge state



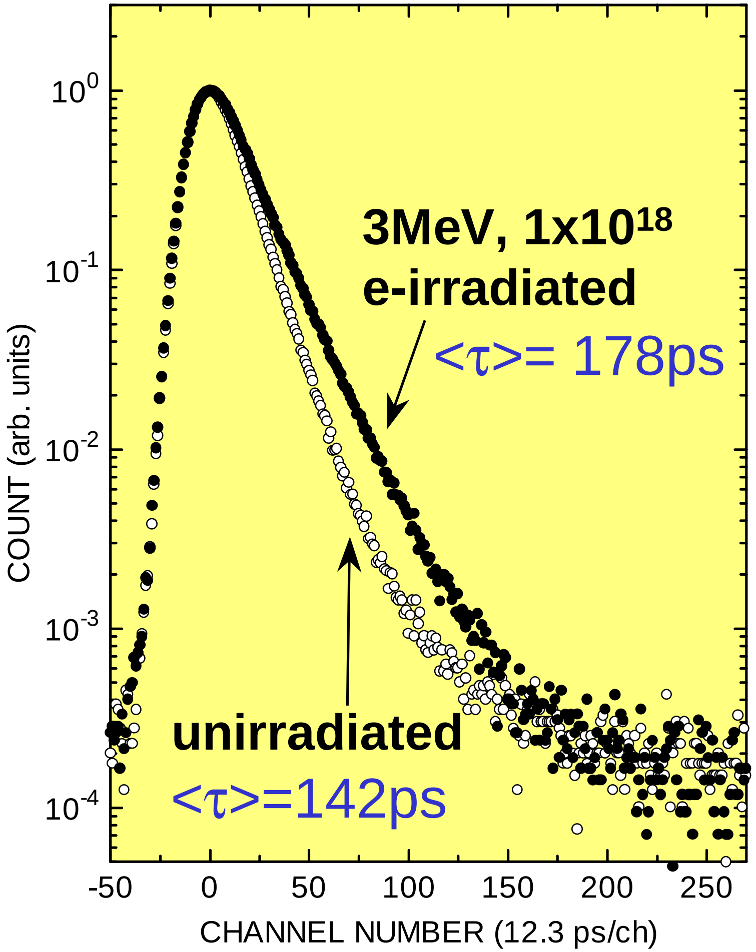


$k_BT \sim Ze^2/4\pi\varepsilon r$

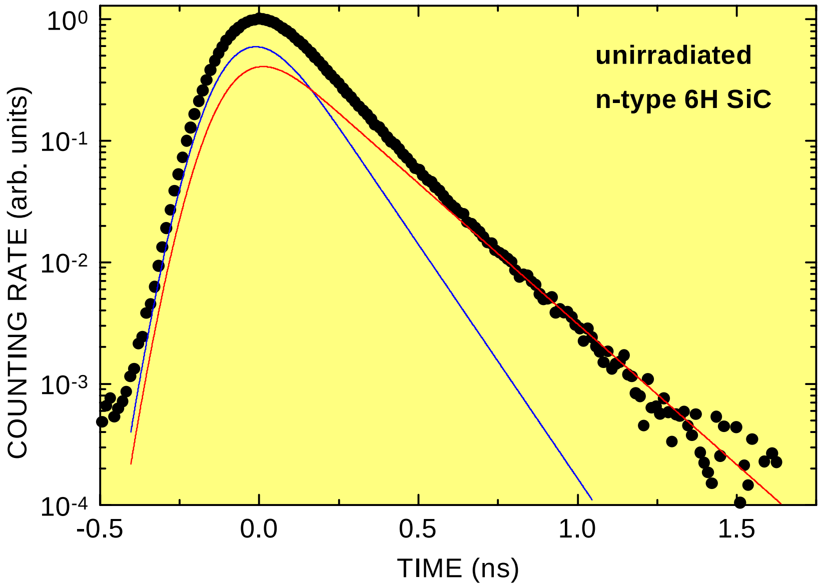
Dielectric constant **ε**

6.7 (SiC) < 11.9 (Si)

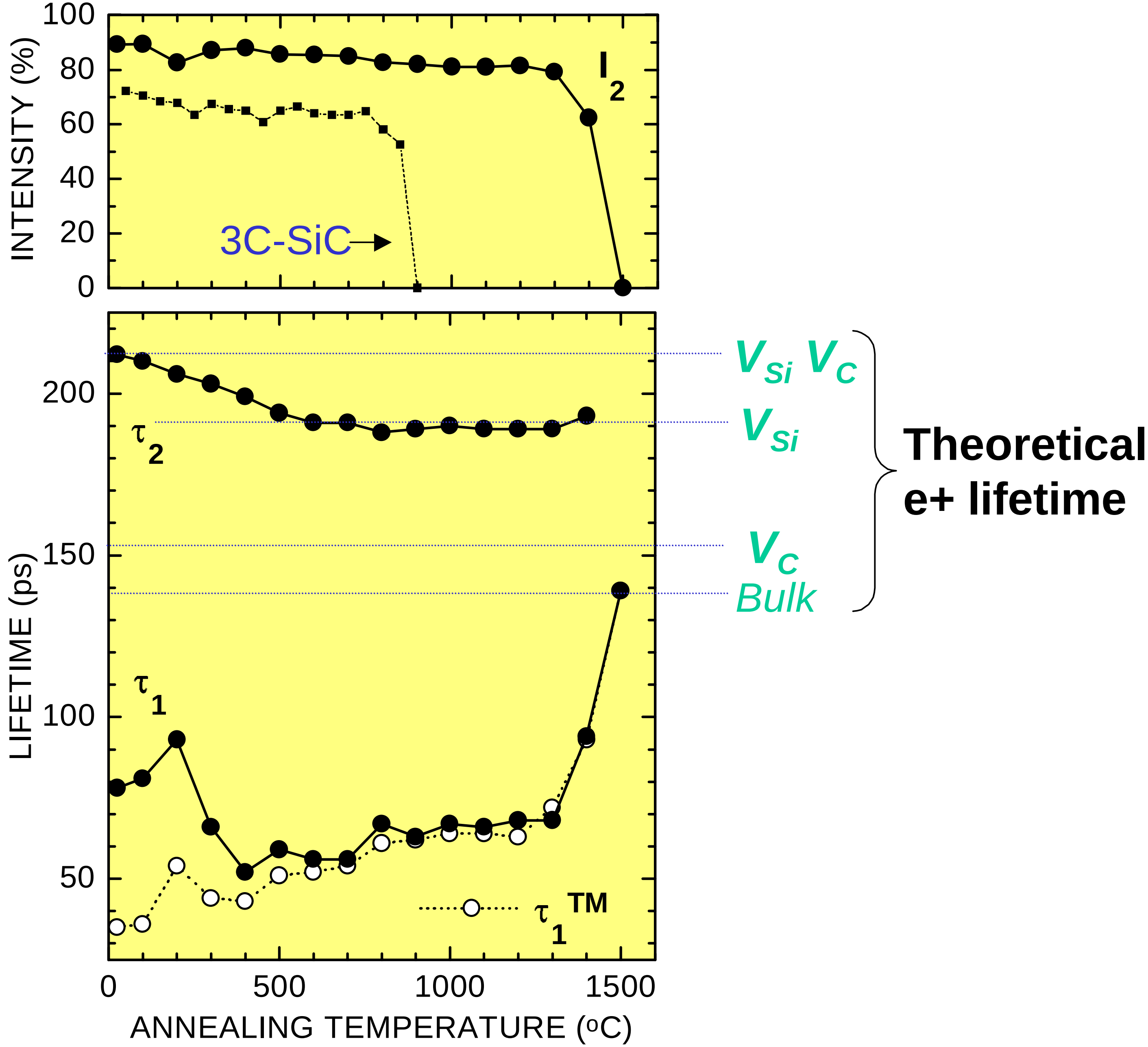
e-irradiated n-type 6H-SiC (Cree Res.)



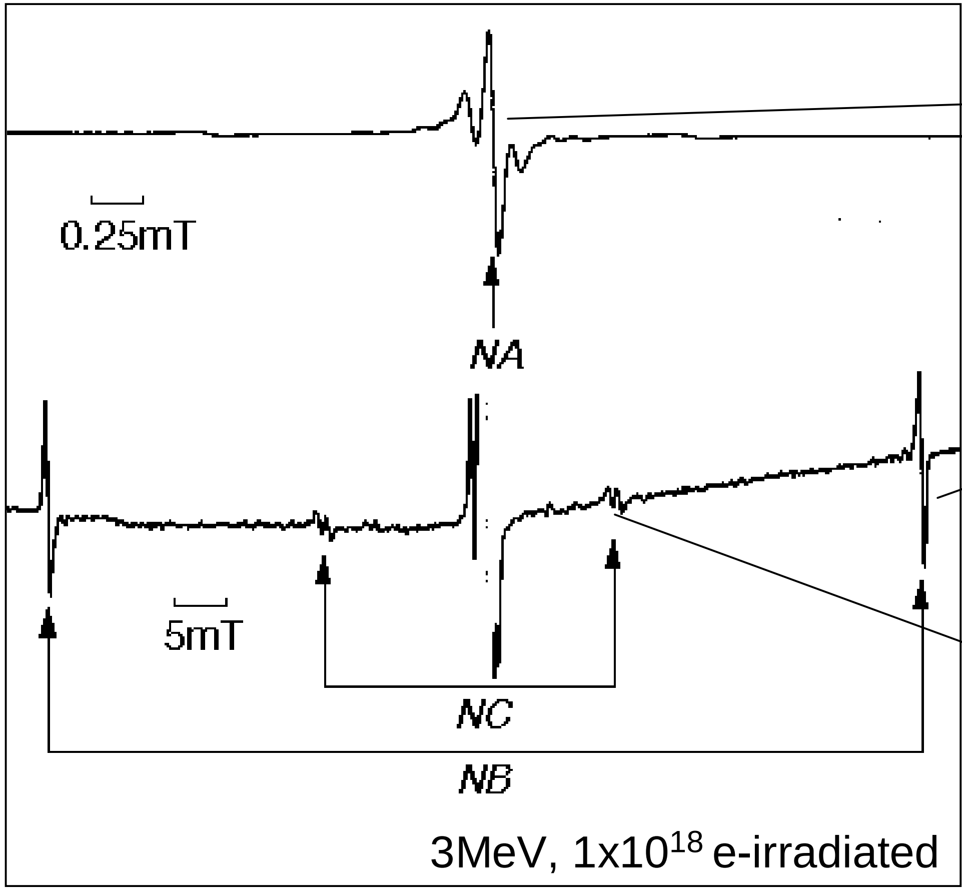
Defects exist in as-grown state



Annealing of e+ lifetime



ESR spectra



NA: g=2.003, isotropic

↕

T1 signal in 3C-SiC

NB: *g*… c-axis symmetry

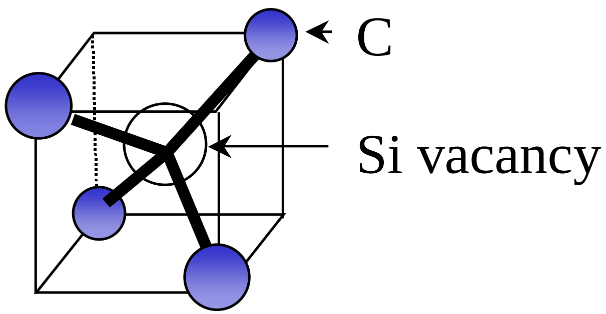
r_{spin}**=4.04A**

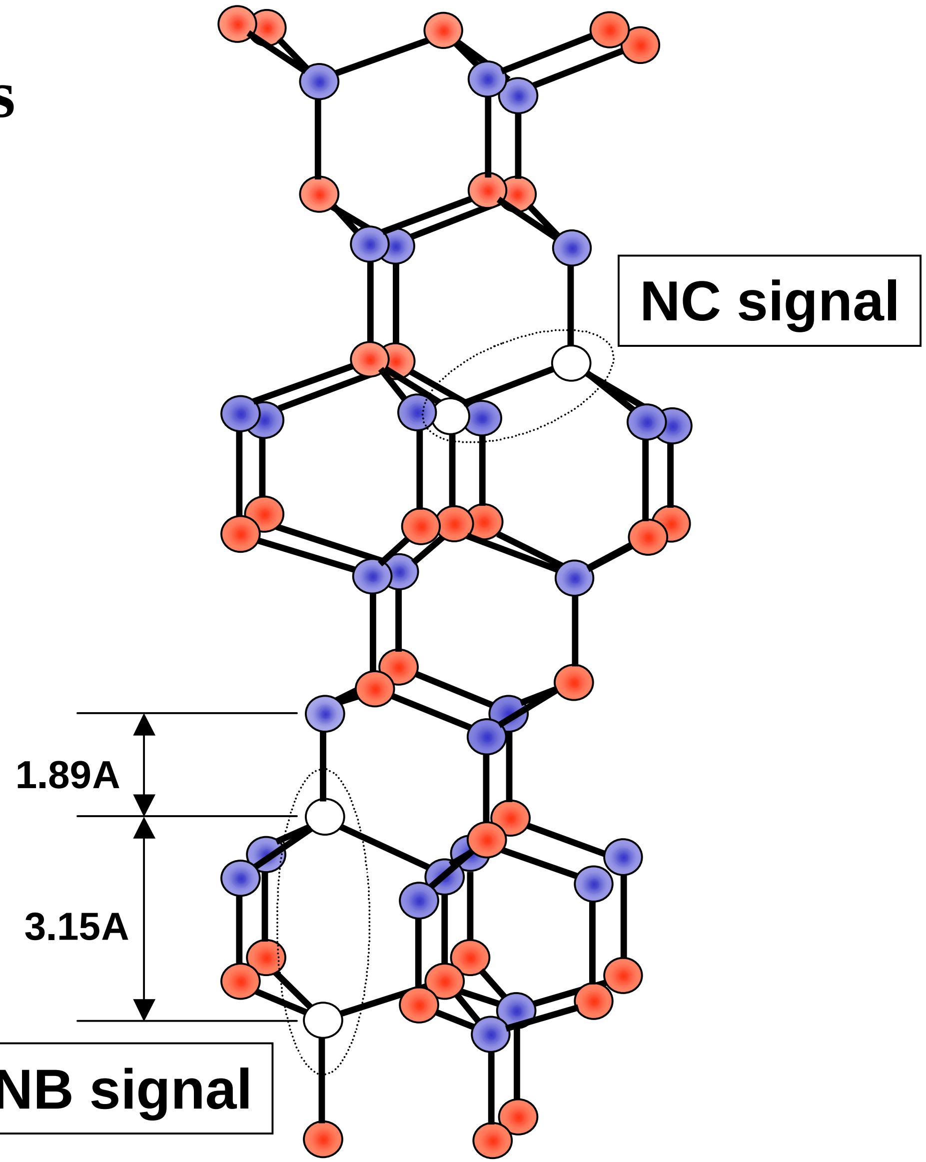
NC: *Principal axes of D deviates ~45º from c-axis*

r_{spin}**=3.62A**

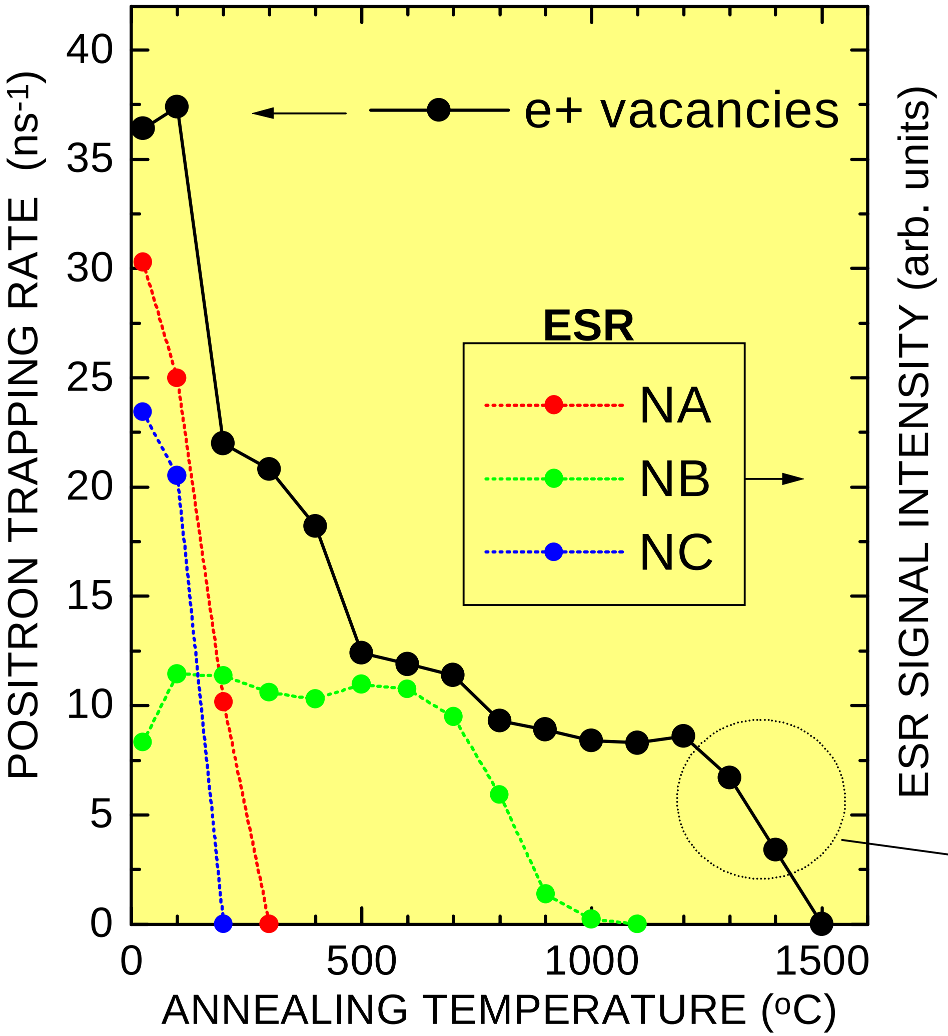
Proposed atomic models for ESR centers

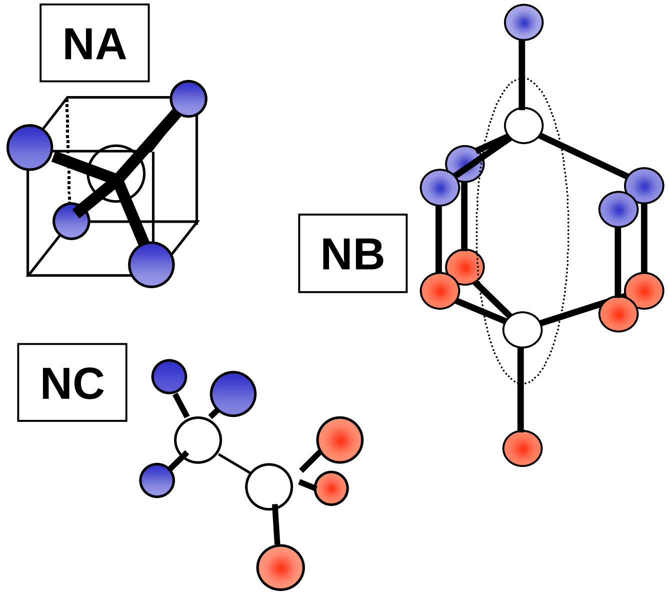
NA signal





e+ detected vacancies and ESR signals

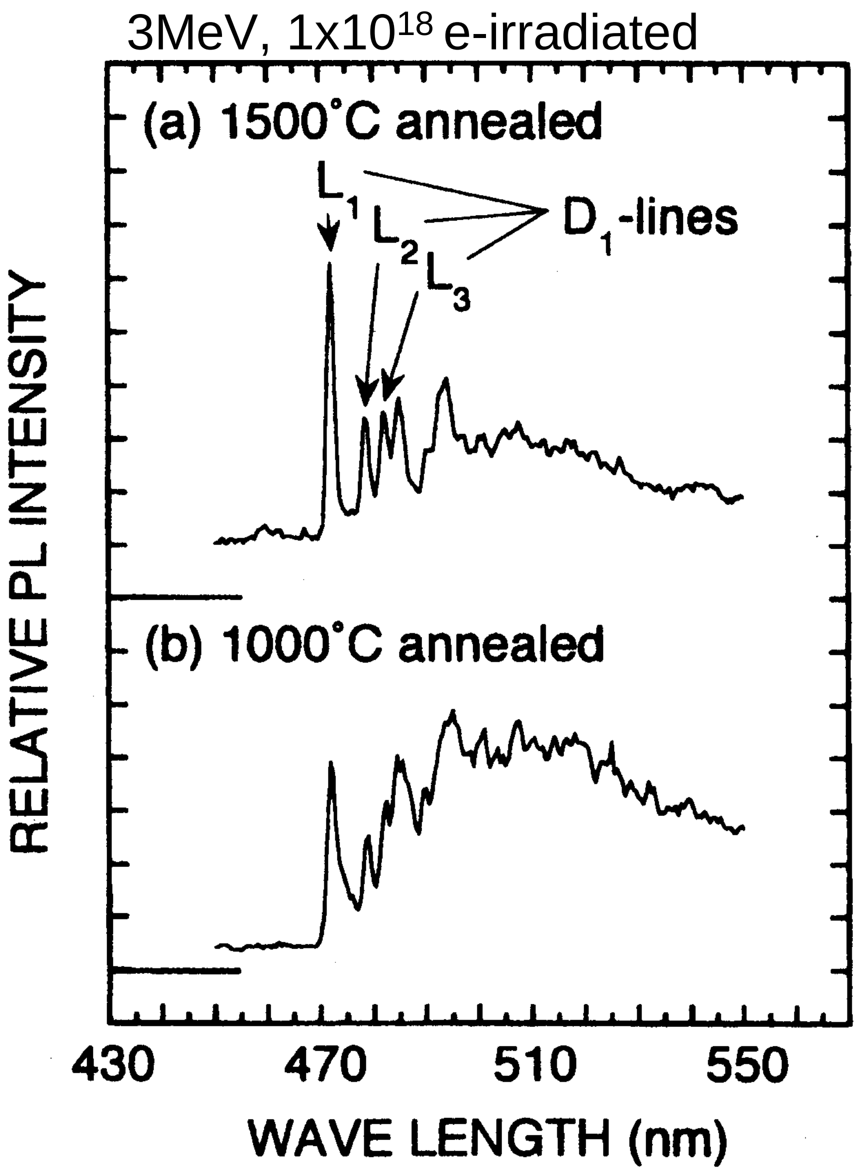




ESR signals are related to vacancy type defects

Related to V_{Si}
e.g.*, V_{si} + *impurities

As for D1 luminescence …

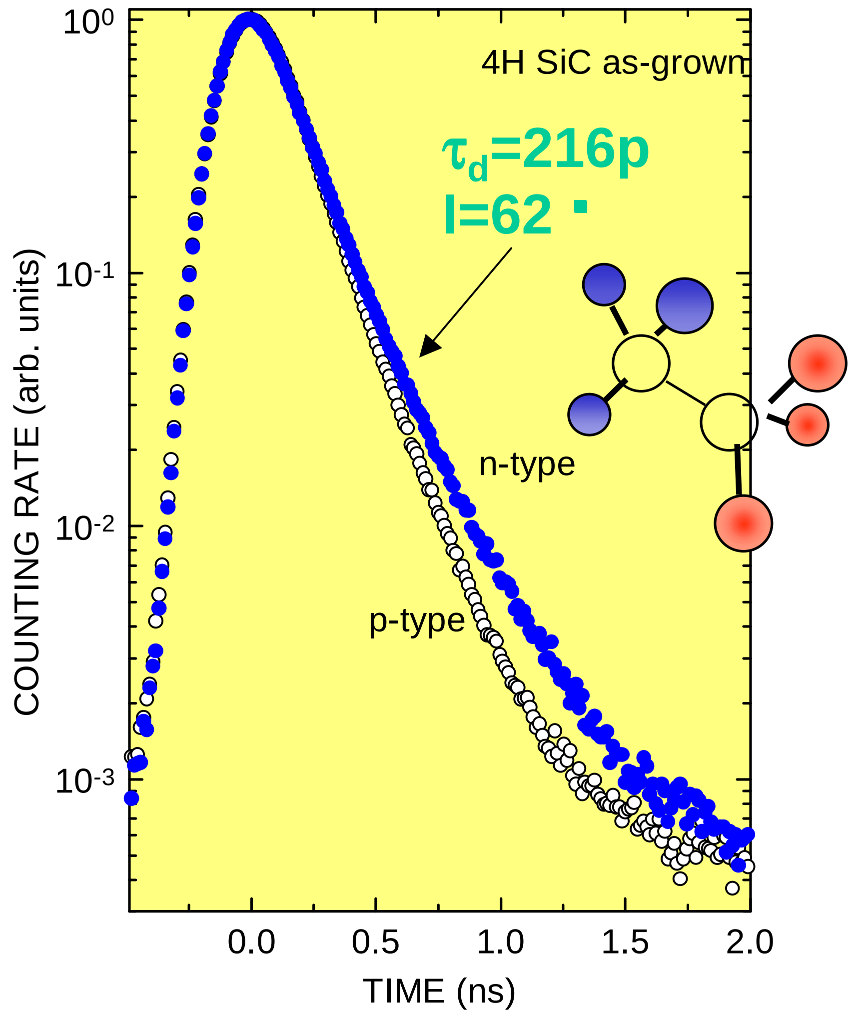


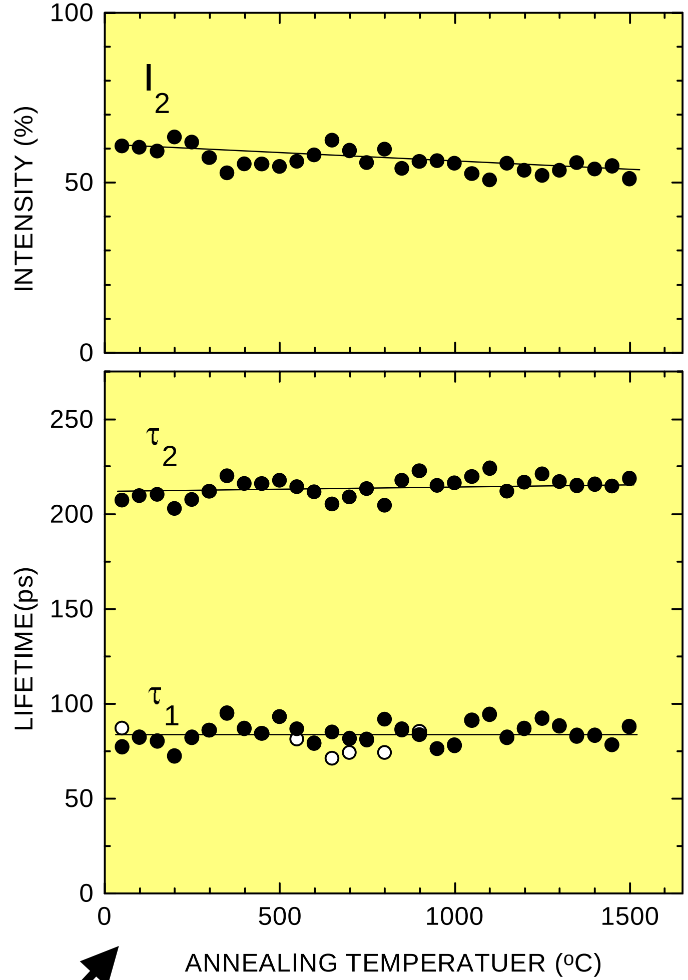
D1 lines remains after 1500°C annealing

×

e+ detected vacancies and ESR centers vanish

4H SiC (Cree Research)





Grown-in vacancies, No change up to 1500ºC

Summary of Part I

Electron-irradiated 3C SiC

- Isolated V_{Si} is major e+ annihilation center.
- Agreement with ESR T1 signal.
- V_{Si} is annealed at 200^{o}C and 800^{o}C.

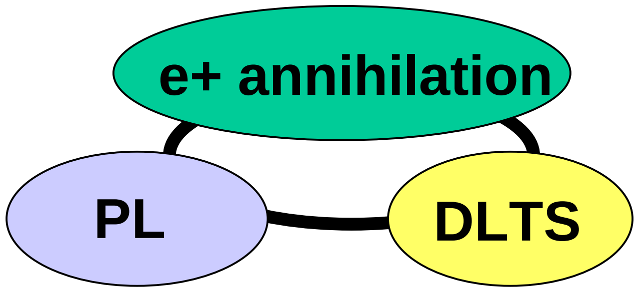
Electron-irradiated 6H SiC

- V_{Si} and $V_{Si}V_{C}$ are e+ annihilation centers.
- ESR NA,NB&NC centers: vacancy type defects.
- No correlation between D1 peaks and e+ detected vacancies

4H SiC

- Grown-in vacancies

Origin of Optical and Electrical Centers



Detailed annealing experiment

High quality epilayer

Conclusions

Positron annihilation is a superior tool to study vacancy-type defects in SiC.

Complementary study of positron and the other methods is necessary to elucidate origin of optical and electrical centers.

Application of positron beam gives us more sophisticated knowledge concerning with defects in epilayers.

Talk is published as pdf-file at:
http://www.ep3.uni-halle.de/positrons/