Surface and bulk radiation induced defects in Si-based sensors

Ioana Pintilie

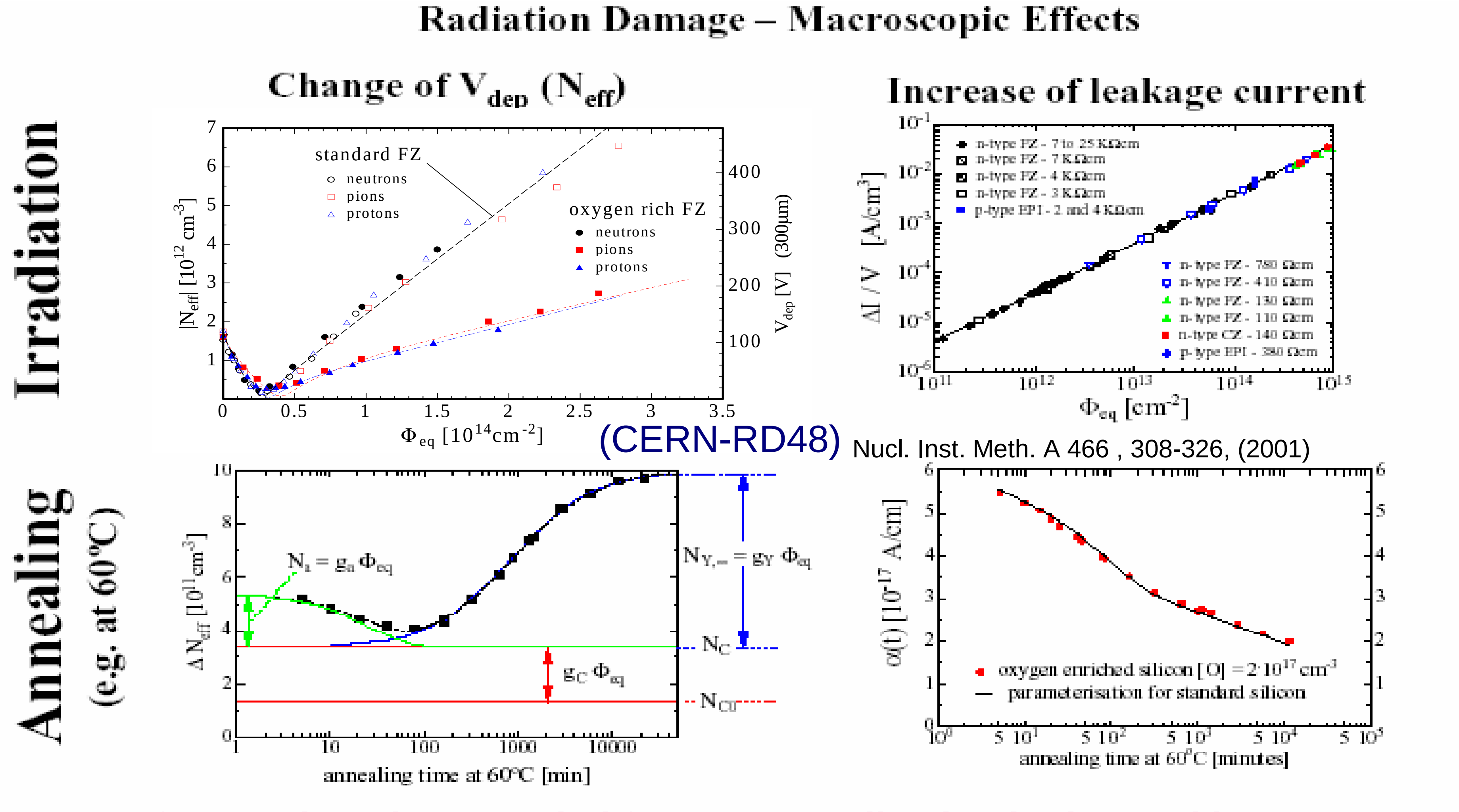
National Institute of Materials Physics, Bucharest, Romania

Outline

- Motivation & Goals
- Electrically active defects
- Bulk radiation damage in Si diodes
- Surface and interface related effects caused by X-rays in Si based MOS capacitors
- Conclusions
- Acknowledgements

Motivation

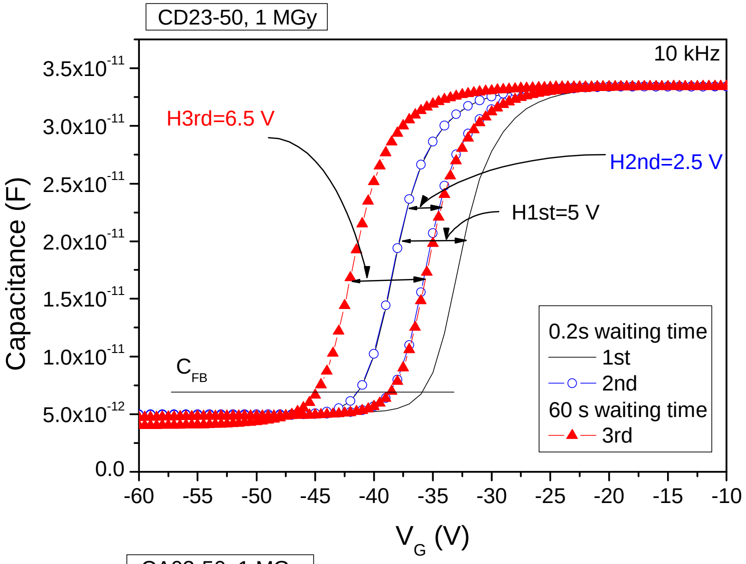
a) *<u>bulk radiation damage</u>* - resulting from the non-ionizing energy loss (as e.g. LHC and SLHC)

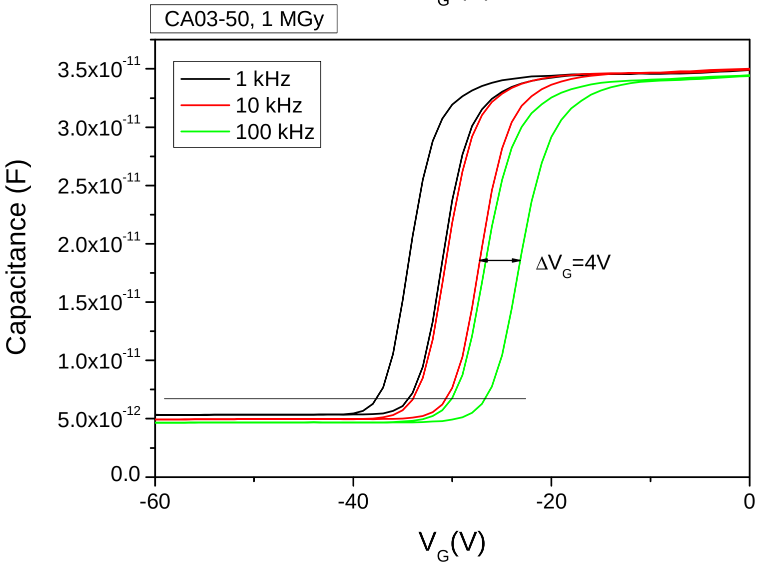


(CERN-RD48) Nucl. Inst. Meth. A 466 , 308-326, (2001)

"Defect engineering" needed for SLHC application in the tracking area to improve the detectors radiation tolerance

b) *Surface and interface related effects* - caused by ionization in environments with high X-ray doses (as e.g. in XFEL).





MOS with high resistivity Si (for XFEL)

- Irreproducibility of C/G-V curves (V_{FB} depending on frequency and on bias history)
- Strong annealing effects at room temperature
- No existing data related to electrical parameters of interface states

Defect investigations needed to understand and predict the performance of segmented Si sensors as a function of the X-ray dose

Goals

- Search for still undetected defects responsible for the radiation damage, as seen at operating temperatures

Bulk defects:

  - Atomic point defects, predominant after gamma and electron irradiation
  - Extended defects (clusters), responsible for hadron damage

Surface defects:

  - Interface states
  - Oxide states

Electronic point defects (e.g after 12 keV X-rays)

- Understand the defect generation and kinetics in order to predict and to optimize the device performance

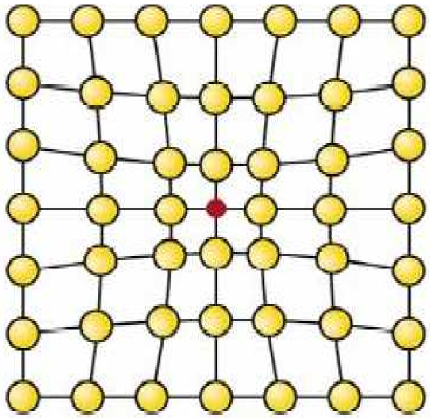
• Electrically active defects

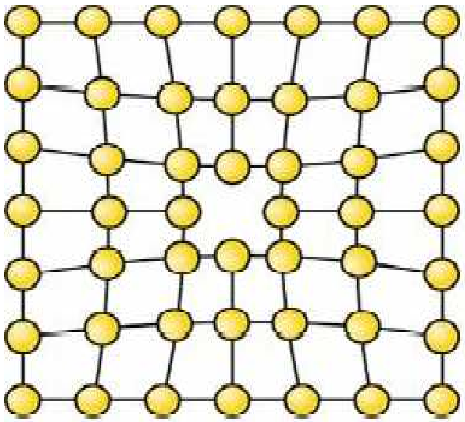
Atomic point defects

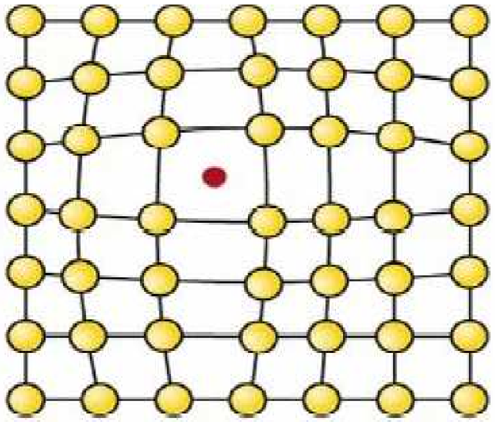
Radiation induced

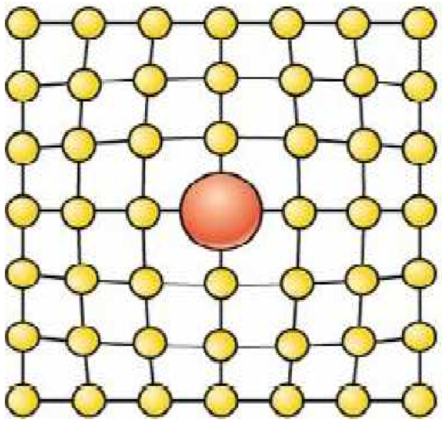
<u>vacancy</u>
- missing atom

<u>interstitial atom</u>
- not in regular lattice site





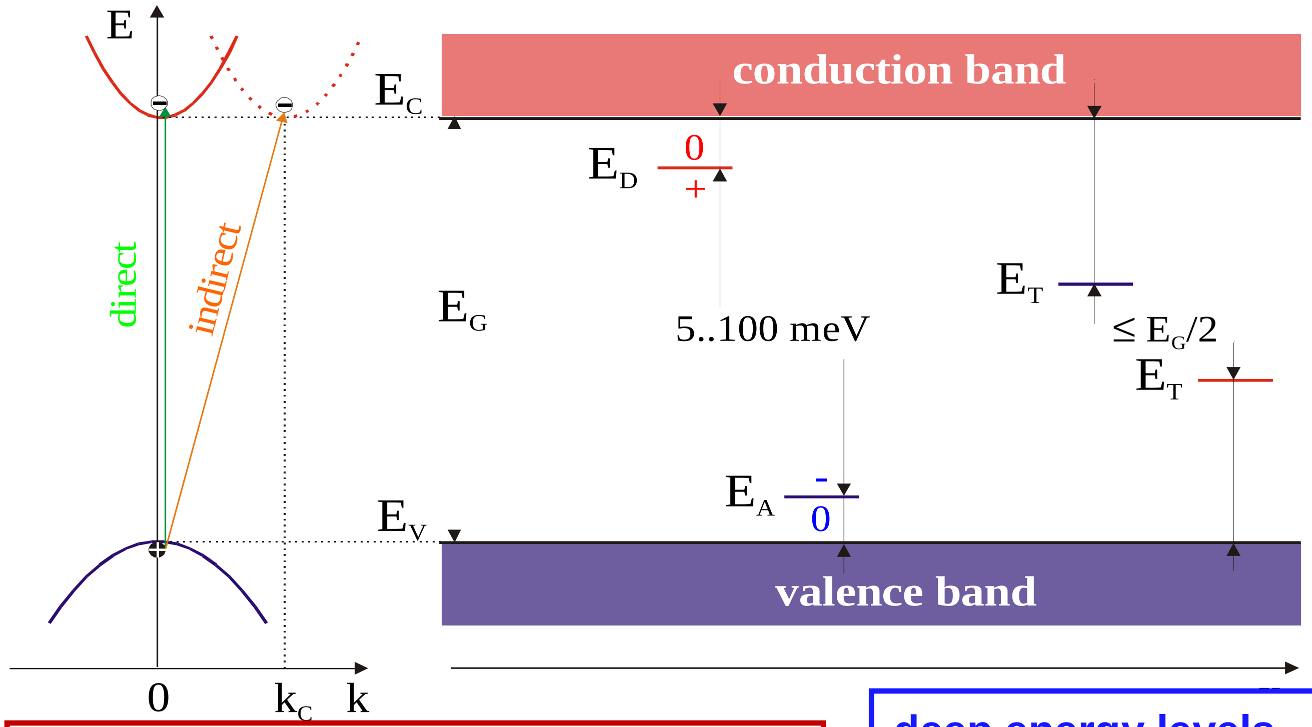




<u>Complexes</u> can form between different kinds of defects

- Local distortion of the crystalline structure
- Some defects may introduce energy levels in the band-gap of the material (electrically active defects)

Clasification of electrically active defects



Donors (0/+)

Deep trapping centers (acceptor or donor like)

Acceptors (-/0)

shallow energy levels

- single impurity atoms - doppants
- Donors, acceptors (e.g. Si: P or B)

➢ adjustment of conductivity,

n- or p-type

deep energy levels

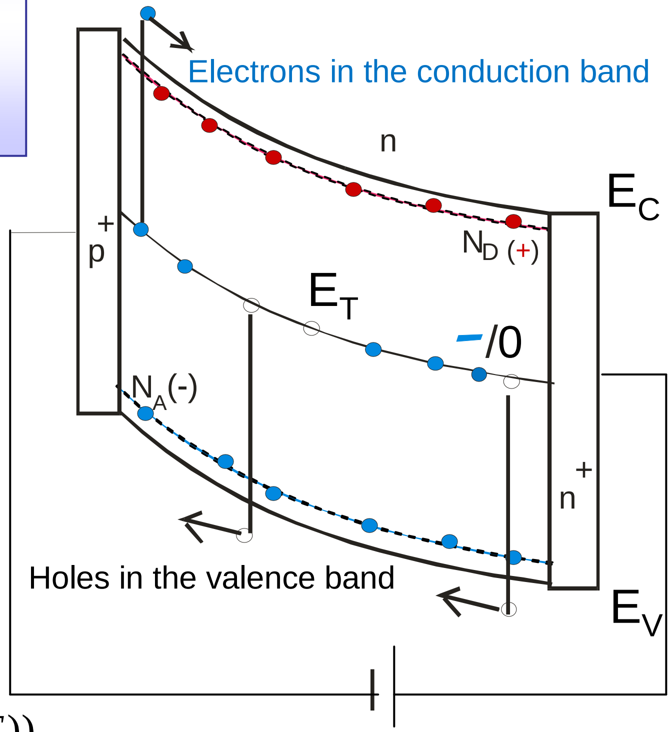
- TM impurities or complex defects (intrinsic defects, radiation induced defects)
- recombination, generation or compensation

➢ even in low concentration deterioration of device characteristics (p-n junction)

Electrical properties of Point Defects - in the Space Charge Region (SCR)

Defect´ signature – emission rates

$$e_{n,p}(T) \sim \sigma_{n,p}(T) * \exp\left(\pm \frac{E_T(T)-E_{C,V}}{k_b T}\right)$$



1) **Contribution to $\mathbf{N_{eff}}$** - given by the steady state ocupancy of the defect levels in SCR

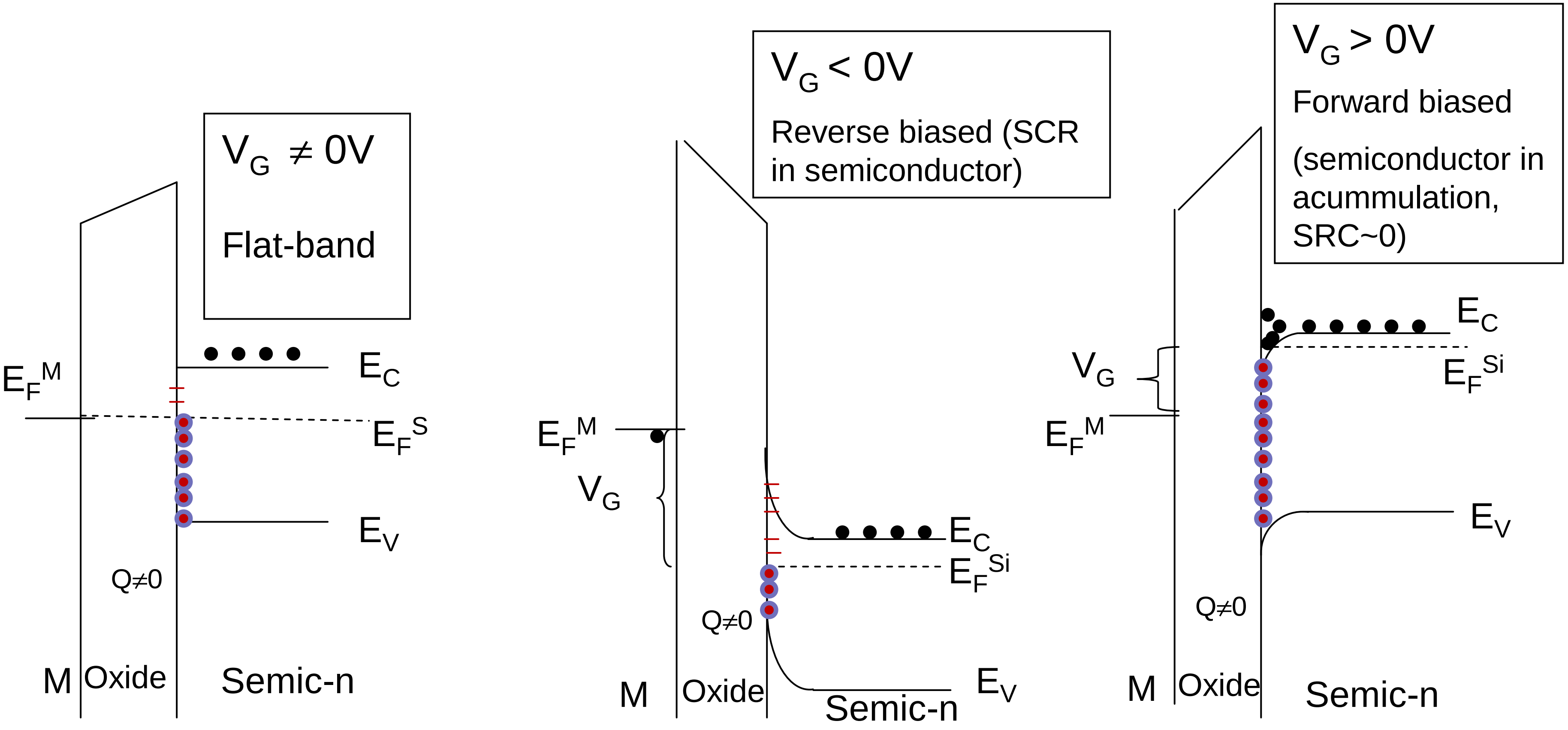
$$n_T^{acceptor}(T) = N_T \frac{e_p(T)}{e_n(T)+e_p(T)}; n_T^{donor}(T) = N_T \frac{e_n(T)}{e_n(T)+e_p(T)}$$

$$N_{eff} = \sum n_T^{donor} - \sum n_T^{acceptor}$$

2) **Contribution to the leakage current**

$$I_{dep}(T) = q_0 * A * d * \left(\sum e_n(T) * n_T^{acceptor}(T) + \sum e_p(T) * n_T^{donor}(T)\right)$$

- *in MOS like structures*



$V_G \neq 0V$

Flat-band

$V_G < 0V$

Reverse biased (SCR in semiconductor)

$V_G > 0V$

Forward biased

(semiconductor in acummulation, SRC~0)

Capacitance-Voltage characteristics in MOS structures

Interface capacitance - C_{it}

$$C_{it}(\Psi_s)=\frac{q^2}{kT}\cdot A\cdot\int_0^{E_g} D_{it}(E_t)\cdot\frac{f_t^0(1-f_t^0)}{(1+\omega^2\tau^2)}\cdot dE_t$$

$$f_t^0(\Psi_s)=\frac{1}{1+e^{\frac{-\Delta E_t-q\psi_s-E_F}{kT}}}$$

$$\tau=\frac{1}{\sigma_n v_{th} N_d}\cdot\frac{1}{\left(e^{\frac{q\Psi_s}{kT}}+e^{\frac{-\Delta E_t-E_F}{kT}}\right)}$$

Charge on interface states - Q_{it}

if acceptors

$$Q_{it}^{A0}(\psi_s)=-q\cdot A_{ox}\cdot\int_0^{E_g} D_{it}(E_t)f_t^0(E_t,\psi_s)dE_t$$

if donors

$$Q_{it}^{D0}(\psi_s)=q\cdot A_{ox}\cdot\int_0^{Eg} D_{it}(E_t)(1-f_t^0(E_t,\psi_s))dE$$

E.H. Nicollian, J.R. Brews, MOS – Physics and Technology, Wiley, 1982

$$C(\Psi_s,\omega)=C_{ox}\cdot\frac{C_{it}(\Psi_s,\omega)+C_S(\Psi_s)}{C_{ox}+C_{it}(\Psi_s,\omega)+C_S(\Psi_s)}$$

$$V_G(\Psi_s)=\Psi_s-\frac{Q_{ox}}{C_{ox}}-\frac{Q_S(\Psi_s)}{C_{ox}}-\frac{Q_{it}(\Psi_s)}{C_{ox}}$$

Interface states – influence the Capacitance/Conductance shape and the frequency dependence

Oxide states – direct influence on flat-band voltage

Methods of Detection – there is no experimental method to provide all the defects characteristics

Technique	**Based on**	**Defect parameters**	**Limitations**
Deep Level Transient Spectroscopy	Charge capture/emission - Capacitance transients	E_t, $\sigma_{n,p}$, N_t	-low density of defects (<10^{12} cm^{-3}) -Chemical nature (indirect)
Thermally Stimulated Current (TSC) /Thermally Dielectric Relaxation Current (TDRC)	Charge capture/emission – Current	E_t, $\sigma_{n,p}$, N_t	-medium density of defects (10^{12} -10^{15} cm^{-3}) -Chemical nature (indirect)
Photoluminescence	Photon Absorption followed by Photon Emission (Luminescence)	PL bands (E_t, τ)	-Only for radiative recombination centers - Chemical nature (indirect) - E_t, $\sigma_{n,p}$, N_t
Infrared Spectroscopy	Absorption of infrared energy on vibrational modes of molecules	-N_t (acc. 20-30%) - Information about structure	-Large density of defects (> 10^{15} cm^{-3}) -E_t, $\sigma_{n,p}$,
Electron Paramagnetic resonance	Zeeman effect and Spins resonance - microwave photons absorption	- Chemical nature and vecinity - N_t	-Large density of defects (> 10^{12} cm^{-3}) - Only paramagnetic centers - E_t, $\sigma_{n,p}$,

• Bulk radiation damage in Si diodes

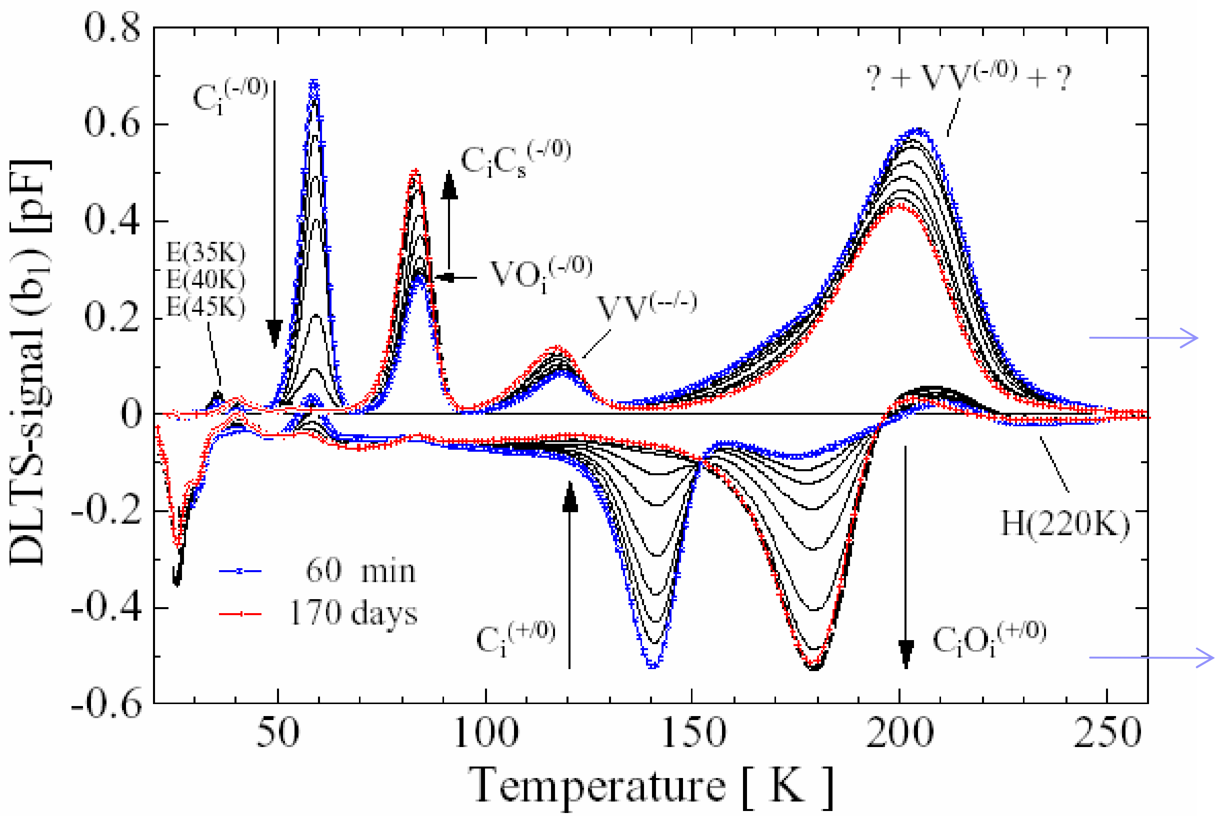
Material

- **Float zone- Silicon wafers: <111>, 300 μm, 3-4 kΩcm, N_d~10^{12} cm^{-3}**
  - standard Oxidation (STFZ) - N_d~$8x10^{11}$ cm^{-3}
  - difusion oxygenated (72 h at 1150 C) (DOFZ) N_d~$1.2x10^{12}$ cm^{-3}
- **MCz-Silicon wafers: <100>, 300 μm, 870 Ωcm, N_d = $4.94x10^{12}$ cm^{-3}**
- **EPI-Silicon wafers: <111>**
  - **25 and 50 μm on 300 μm Cz-substrate, 50 Ωcm, N_d~$7.2x10^{13}$ cm^{-3}**
  - **75 μm on 300 μm Cz-substrate, 169 Ωcm**
    - standard Oxidation (EPI-ST), N_d = $2.66x10^{13}$ cm^{-3}
    - diffusion oxygenated for 24 h/1100℃ (EPI-DO) N_d = $2.48x10^{13}$ cm^{-3}

Irradiations

- **Co^{60} γ-source** at BNL, dose range 1 to 500 Mrad
- **6 -15 MeV electrons**: irradiation facility at KTH Stockhom, Sweden
- **23 GeV protons**: irradiation facility at CERN
- **1 MeV neutrons**: TRIGA reactor in Ljubljana/Slovenia

Si diodes – *typical DLTS spectra*
(low irradiation fluence)



Electron traps

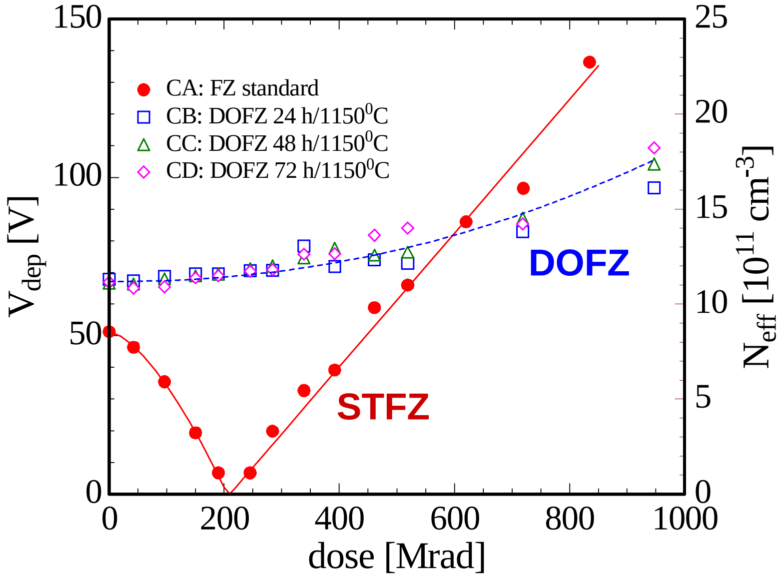
Hole traps

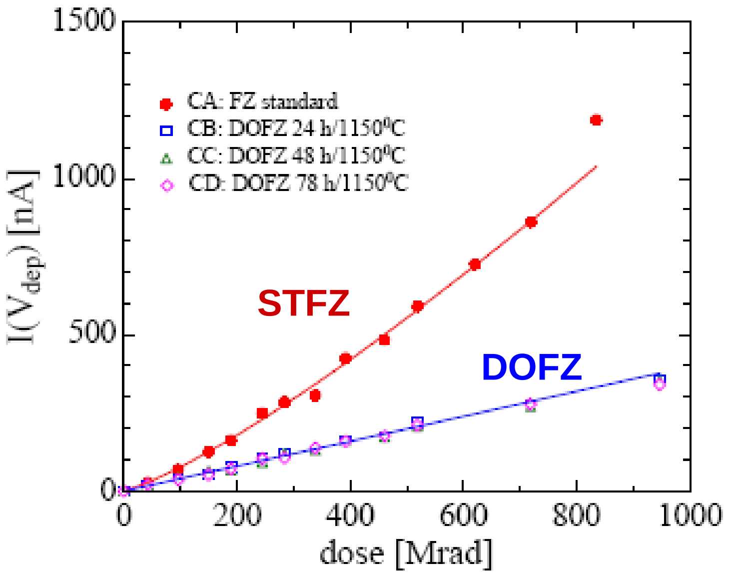
Phys. Rev. B **13, 2653 , (1976);** Radiat. Eff. **29, 7, (1976);** J. Appl. Phys. **79, 3906, (**1996); Nucl.Instrum. Methods Phys. Res. A **388, 335 , (1997);** M. Moll, Ph.D. thesis, DESY thesis 1999-040, ISSN 1435-8085, 1999

None of these defects explain the macroscopic behaviour of the irradiated diodes

Results – Point Defects

Co^{60}- γ irradiation – only point defects are generated

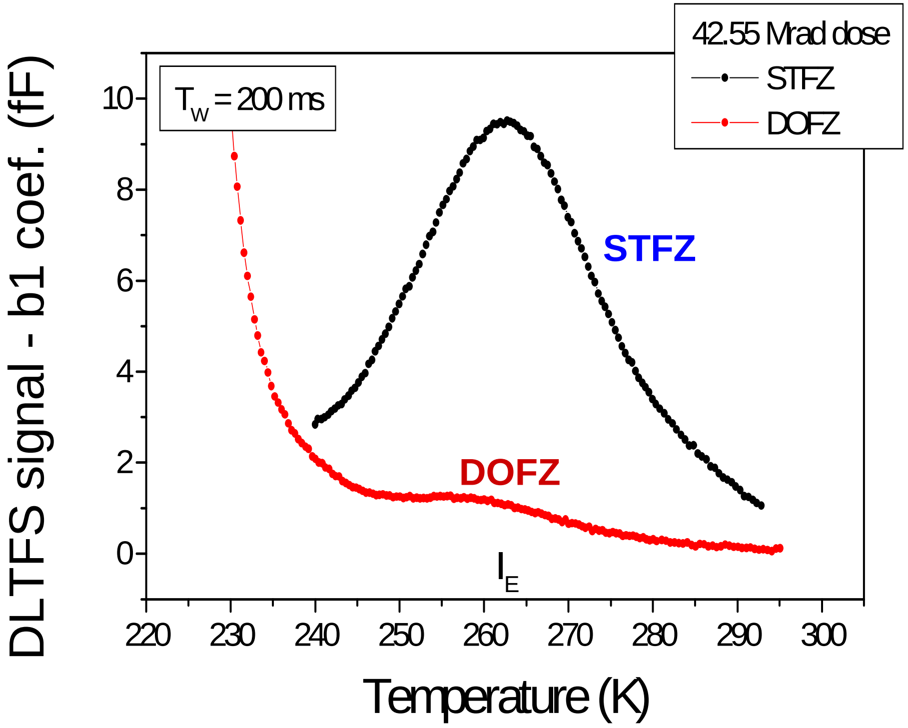




- **Very pronounced beneficial effect of oxygen on both I and V_{dep}**
- ***Close to midgap acceptor correlated with [O] responsible ?***

Nucl. Inst. Meth. A 514 (2003) 1–8

- Low irradiation γ doses (but already high for DLTS)



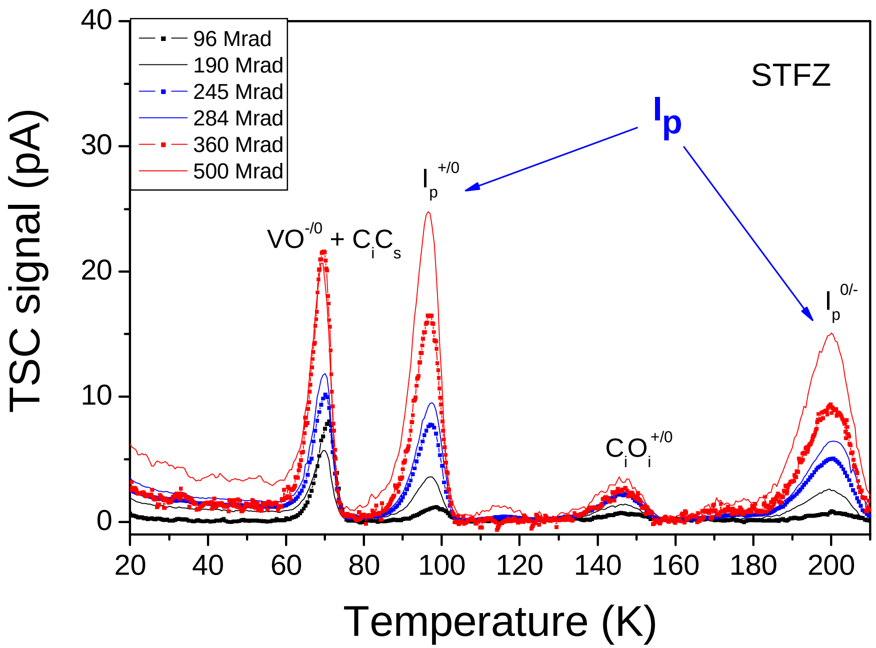
APPLIED PHYSICS LETTERS 81 , 165-167, 2002

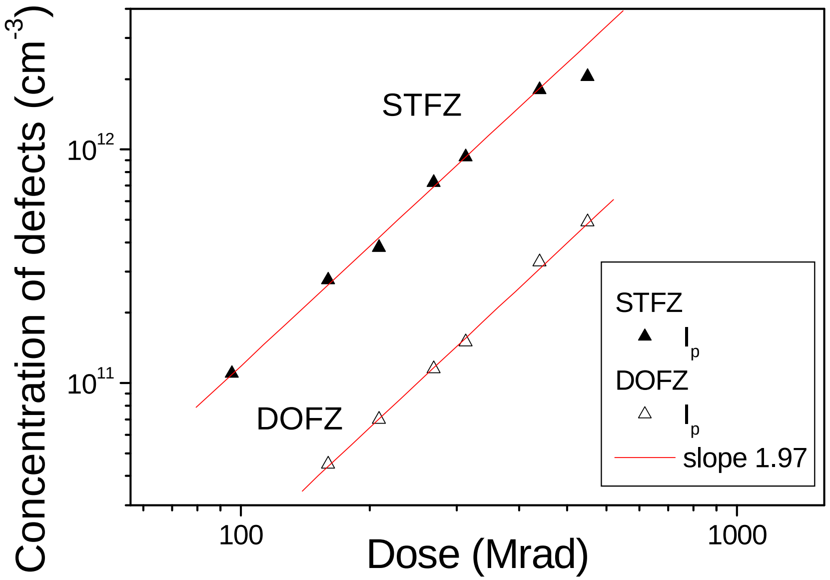
I_p center

- ***deep acceptor*** (-/0)
- Ea = Ec – 0.545 eV
- $\sigma_n = (1.7 \pm 0.2) \times 10^{-15}$ cm^2
  - direct measurement
- $\sigma_p = (9 \pm 1) \times 10^{-14}$ cm^2
  - from $N_T^{DLTS}(T)$

~ 90% occupied with (-) at RT

- Higher irradiation γ doses (TSC)





<u>I_p centers</u>

– Two levels in the gap: - a donor E_v+0.23eV (+/0) & an acceptor E_c-0.545 eV (0/-)

- Supressed in Oxygen rich material and Quadratic dose dependence

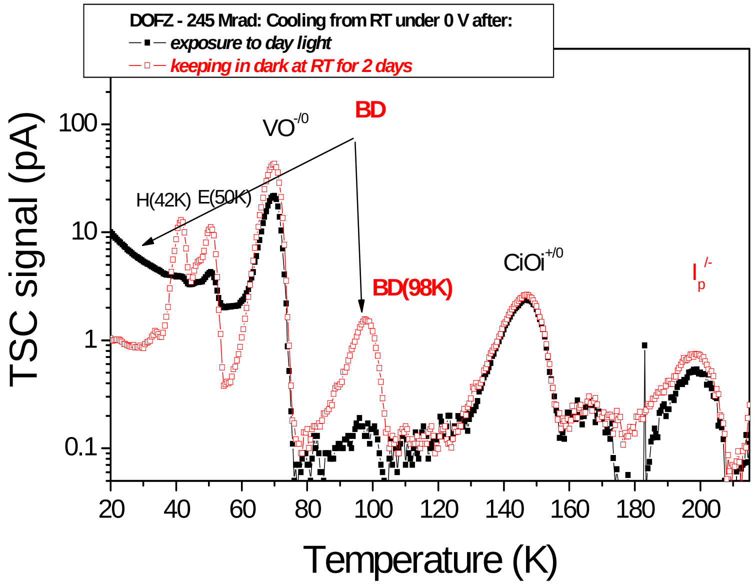
⇒ generated via a 2nd order process (V_2O?) 1) V+O → VO

2) V+VO → V_2O

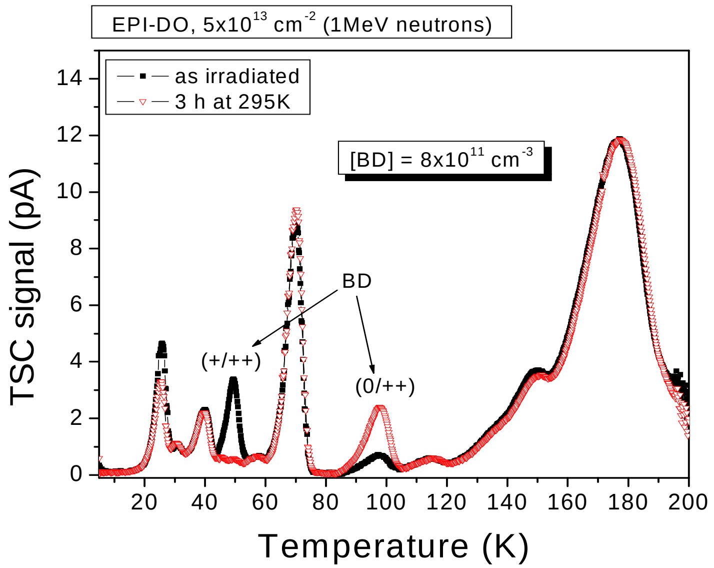
APPLIED PHYSICS LETTERS 82, 2169 (2003); Nucl. Inst. Meth. A 514, 18-24, (2003)

BD center – bistability and donor activity

- In low doped n-type DOFZ



- In medium doped n-type EPI-DO



$E_i^{BD(98K)} = E_c - 0.225\ eV$ (0/++) ; $E_i^{BD(50K)} = E_c - 0.15\ eV$ (+/++)

***BD center** – donor in the upper part of the gap (+ at RT)*

- ***generated in oxygen rich material***
- ***after $C0^{60}$- γ irradiation, can even overcompensate the effect of deep acceptors!***

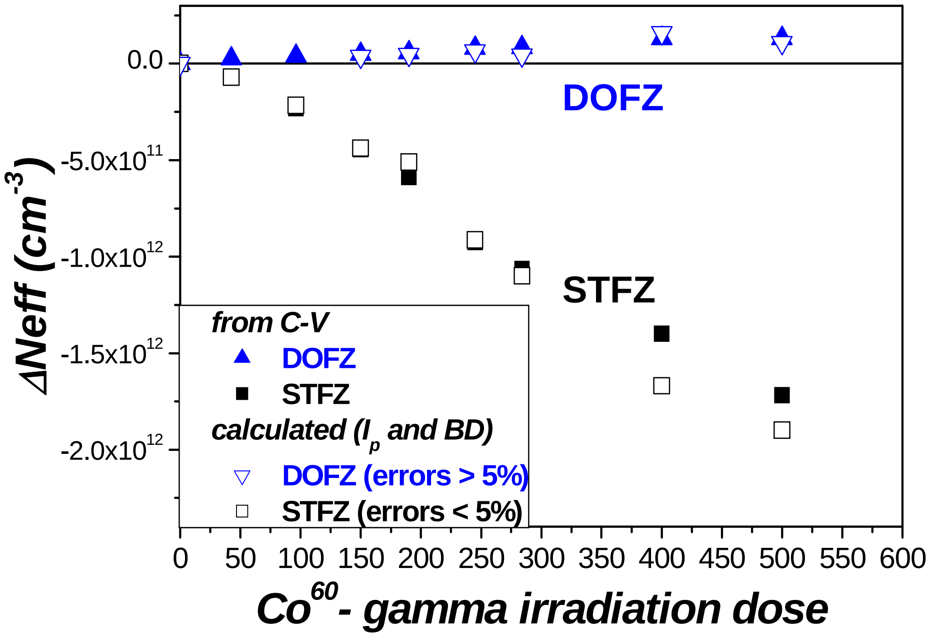
The bistability, donor activity and energy levels associate the BD centers with TDD2 ⇒ oxygen dimers are part of the defect structure

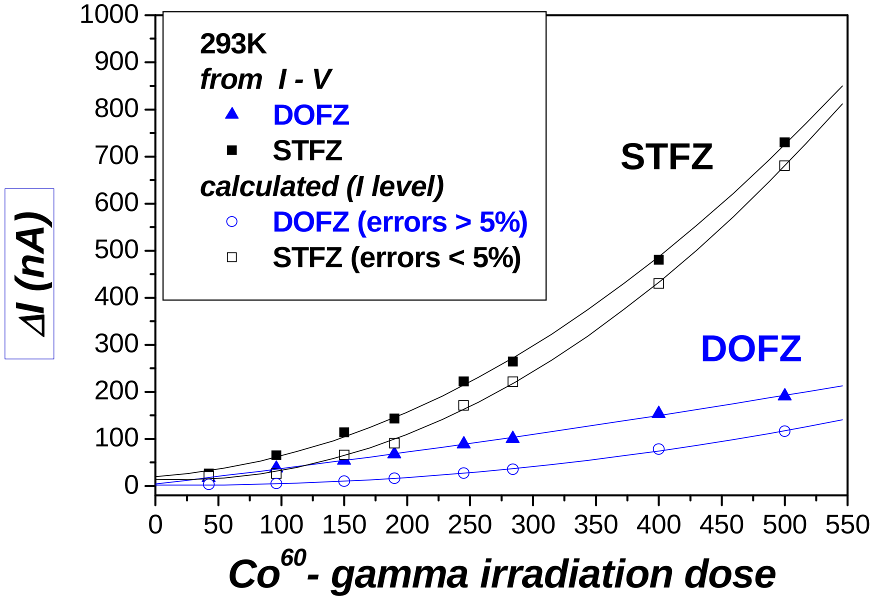
Nucl. Inst. Meth. A 514, 18-24, (2003) ; Nucl. Inst. Meth. A 552 (2005) 56–60; Nucl. Inst. Meth. A 556 (2006) 197–208; Nucl. Inst. Meth. A 583 , 58-63, (2007); Nucl. Inst. Meth. A 611 (2009) 52–68

Impact of I_p and BD defects on detector properties

$$\Delta N_{eff}(T) = -n_T(T)$$

$$\Delta I(T) = q_0 \cdot e_n(T) \cdot n_T(T) \cdot Vol$$





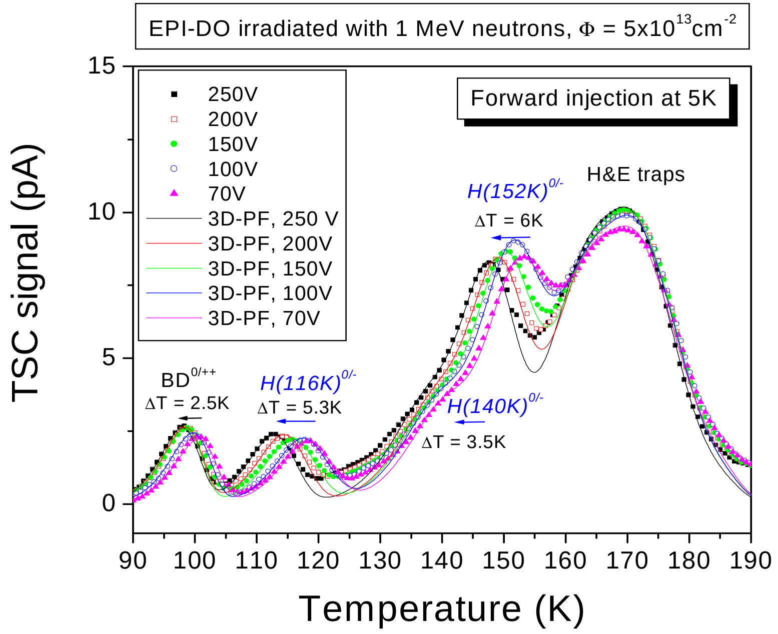
Nucl. Inst. Meth. A 514 (2003) 1-8; Nucl. Inst. Meth. A 611 (2009) 52–68

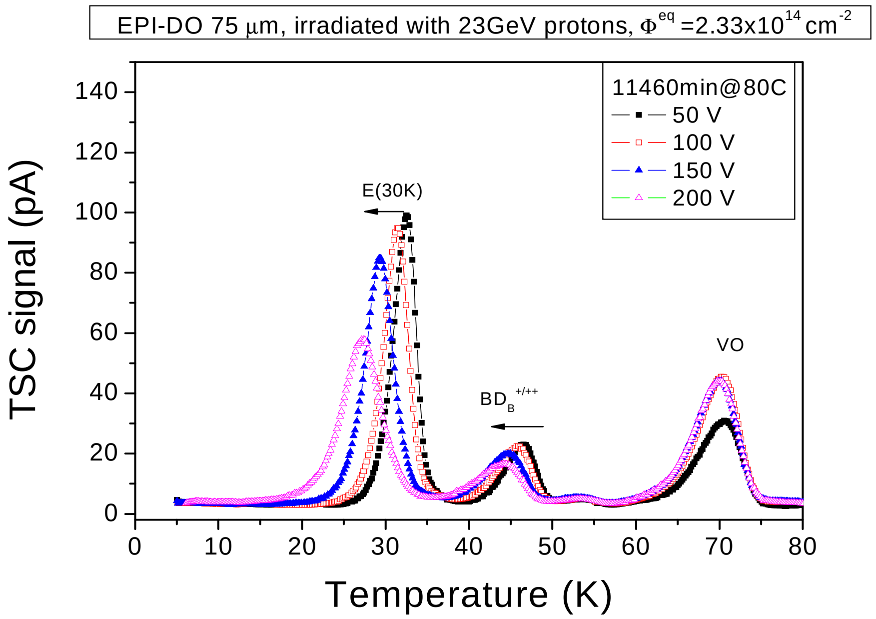
change of N_{eff} and leakage current well described

⇒ first breakthrough in understanding the damage effects

Results – Extended Defects (clusters)

H(116K), H(140K), H(152K) and E(30K) - cluster related traps with enhanced field emission





- The 3D-Poole Frenkel effect formalism describes the experiments

$E_i^{116K} = E_V + 0.33\text{eV}, \sigma_p^{116K} = 4{\cdot}10^{-14}\ \text{cm}^2$
$E_i^{140K} = E_V + 0.36\text{eV}, \sigma_p^{140K} = 2.5{\cdot}10^{-15}\ \text{cm}^2$
$E_i^{152K} = E_V + 0.42\text{eV}, \sigma_p^{152K} = 2.3{\cdot}10^{-14}\ \text{cm}^2$

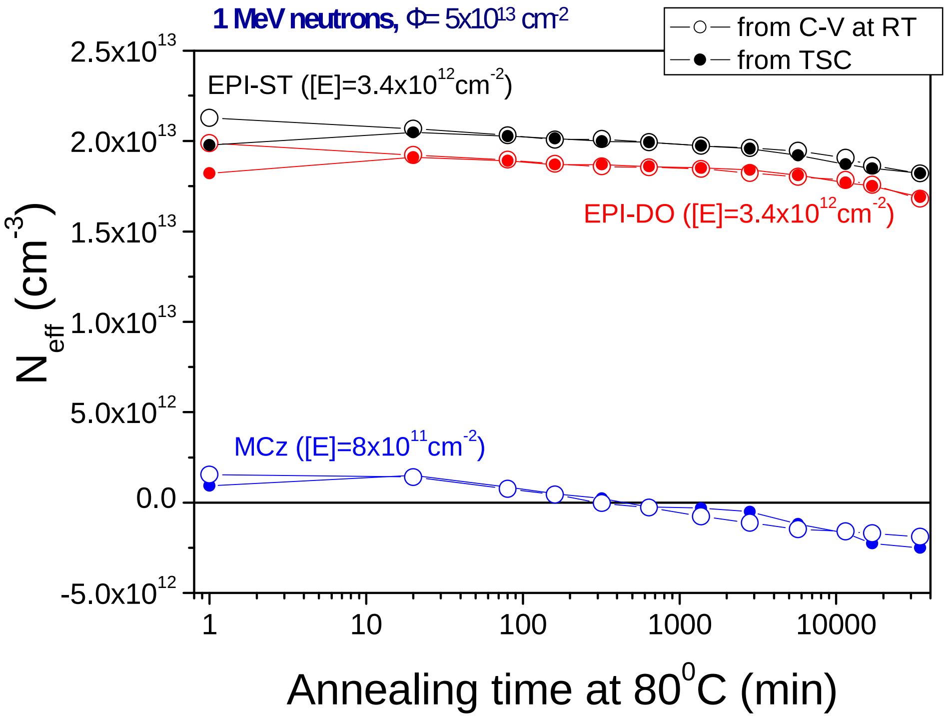
Are acceptors in the lower part of the gap and contribute with (-) space charge at RT

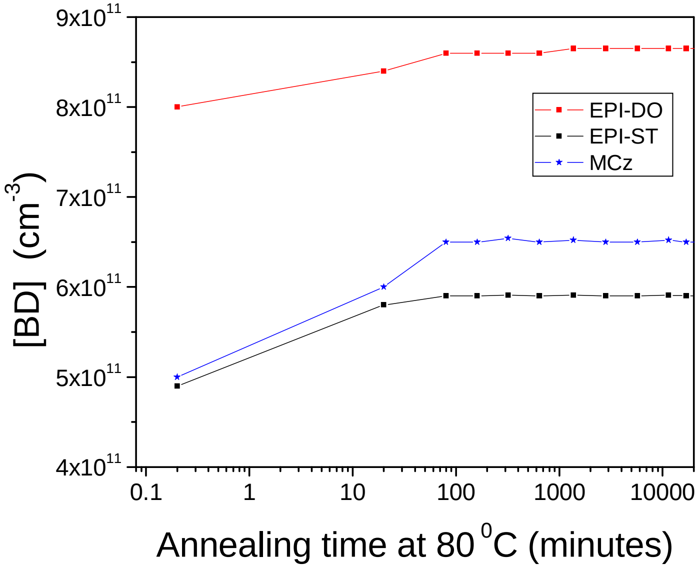
$E_i^{30K} = E_c - 0.1\text{eV}, \sigma_n^{30K} = 2.3{\cdot}10^{-14}\ \text{cm}^2$

Are donors in the upper part of the gap and contribute with (+) space charge at RT and are much more generated after 23 GeV proton irradiation than after 1 MeV neutrons

The impact of BD, E(30K), H(116K), H(140K) and H(152K) on N_{eff}

EPI-ST: $N_d = 2.66\text{x}10^{13}$ cm^{-3}; EPI-DO: $N_d = 2.48\text{x}10^{13}$ cm^{-3}; MCz: $N_d = 4.94\text{x}10^{12}$ cm^{-3}





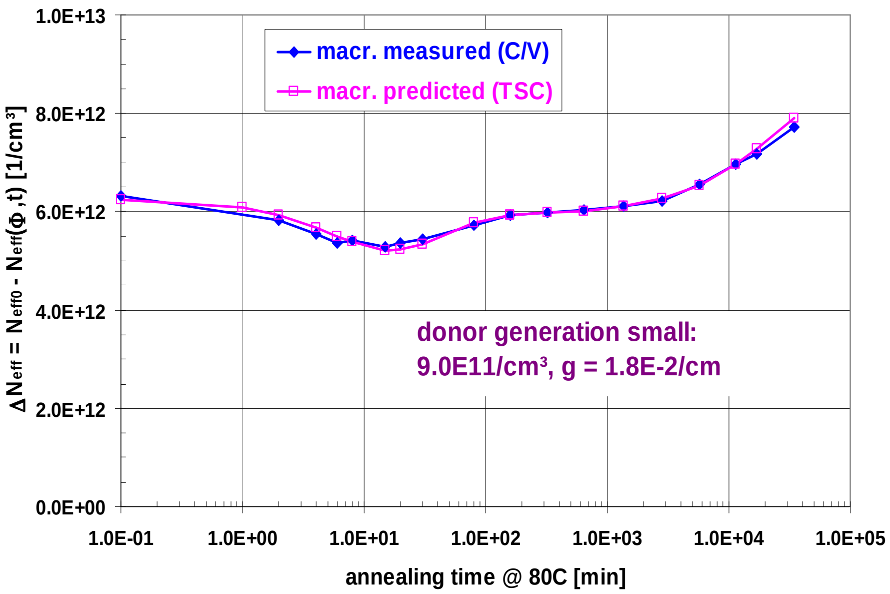
Differences between materials given by the initial doping (N_d) and [BD], only!

⇒ These are the defects responsible for the annealing of N_{eff} at RT!

APPLIED PHYSICS LETTERS **92, 024101 2008;** ; Nucl. Inst. Meth. A 611 (2009) 52–68

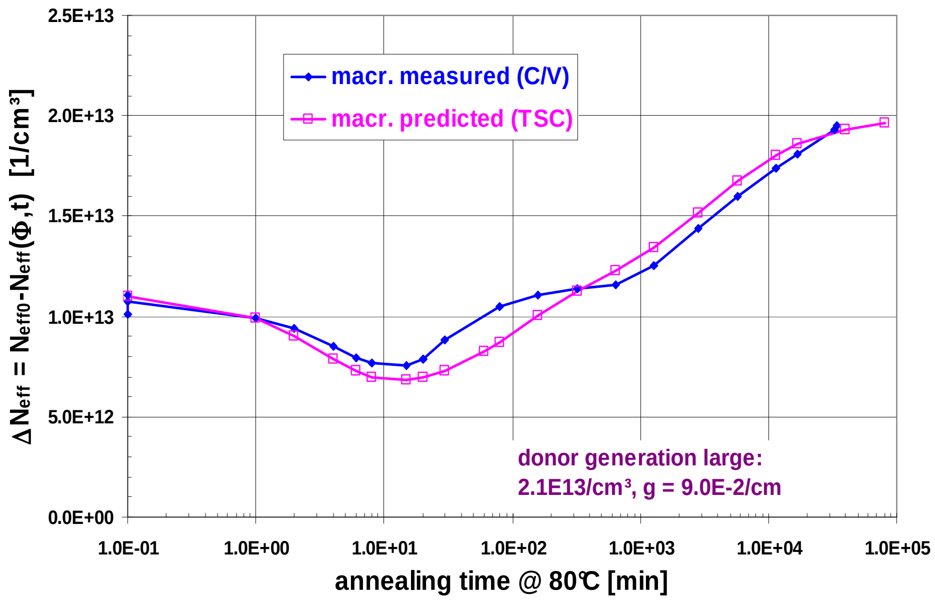
EPI-DO 75 μm: $N_d = 2.48x10^{13}$ cm^{-3}

1 MeV neutrons, $\Phi = 5x10^{13}$ cm^{-2}



donor generation small:
9.0E11/cm³, g = 1.8E-2/cm

23GeV protons, $\Phi_{eq} = 2.33x10^{14}$ cm^{-2}



donor generation large:
2.1E13/cm³, g = 9.0E-2/cm

Larger donor generation (E(30K) and BD) after 23GeV protons than after 1 MeV neutrons (~4.5 times) !

Summary – bulk damage

- Identified point defects induced by irradiation

Defect	$E_{V,C}\pm E_t$ [eV]	$\sigma_{n,p}$ [cm^2]	T_{anneal} [°C]	g [cm^{-1}] N_t/Φ_{eq}	Material
IO_2(-/0)	–0.143	3.8×10^{-14}	≈100	≈ 0.21	MCz, EPI-DO
C_i(-/0)	–0.114	5.9×10^{-15}	≈80		FZ, EPI-ST
$C_iC_s^A$(-/0)	–0.171	1.4×10^{-14}	≈260		FZ, EPI-ST
VO_i(-/0)	–0.176	1.4×10^{-14}	≈300 / >300	0.73	MCz, EPI / FZ
X(=/-) V_2O(=/-)	–0.241	1.1×10^{-14}	≈260 in		MCz, EPI
V_2(=/-)	–0.224	7×10^{-16}	≈260 / 340	0.37	MCz,, EPI / Fz
L, V_3O(=/-)	–0.328	1.23×10^{-15}	≈240 in		MCz, EPI
E4, V_3(=/-)	–0.36	4×10^{-15}	≈240	0.19	MCz, EPI / FZ
E(205a)	–0.393	1.3×10^{-15}	≈180		MCz, EPI / FZ
V_2(-/0)	–0.424	2.1×10^{-15}	≈260 / 340	0.37	MCz, EPI / FZ
X(-/0), V_2O(-/0)	–0.467	1.1×10^{-14}	≈260 in		MCz, EPI
E5, V_3(-/0)	–0.456	5×10^{-15}	≈240	0.19	MCz,, EPI / FZ
C_iO_i(+/0)	+0.360	$2{,}45\times10^{-15}$	≈380	1.3	MCz, EPI / FZ

- not identified defects but with strong impact on the device properties at operating temperature

Point defects

- $E_i^{BD} = E_c - 0.225$ eV
- $\sigma_n^{BD} = 2.3 \cdot 10^{-14}$ cm^2

- $E_i^{I} = E_c - 0.545$ eV
  - ☐ $\sigma_n^{I} = 1.7 \cdot 10^{-15}$ cm^2
  - ☐ $\sigma p^{I} = 9 \cdot 10^{-14}$ cm^2

Cluster related centers

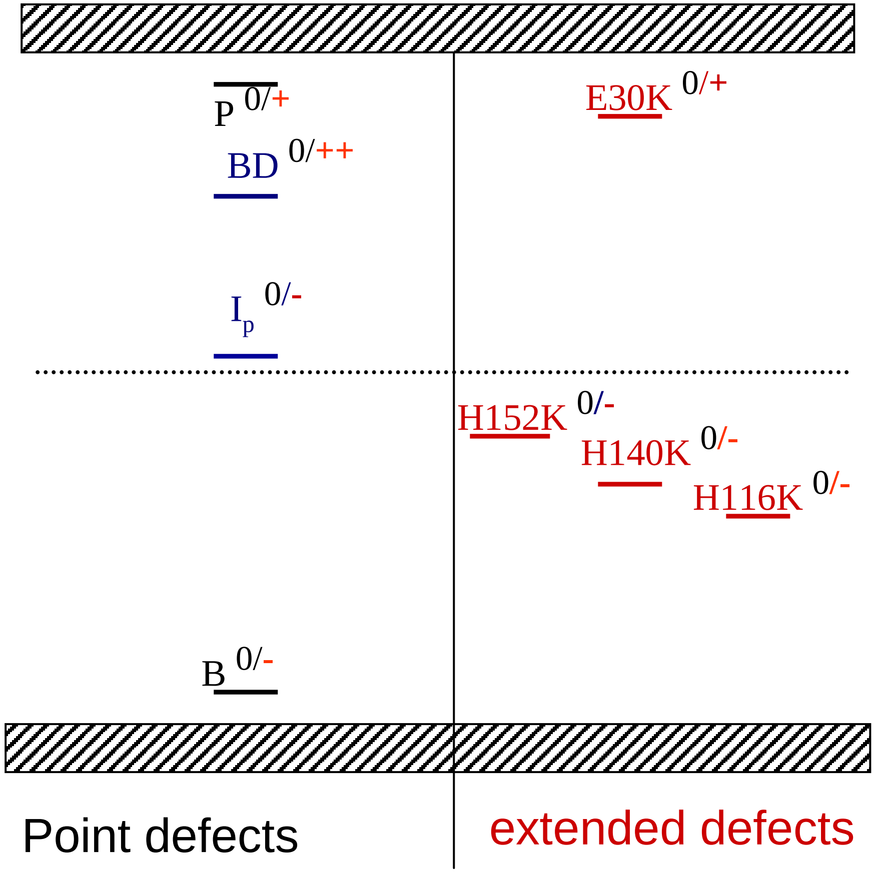
- $E_i^{116K} = E_v + 0.33$eV
- $\sigma_p^{116K} = 4 \cdot 10^{-14}$ cm^2

- $E_i^{140K} = E_v + 0.36$eV
- $\sigma_p^{140K} = 2.5 \cdot 10^{-15}$ cm^2

- $E_i^{152K} = E_v + 0.42$eV
- $\sigma_p^{152K} = 2.3 \cdot 10^{-14}$ cm^2

- $E_i^{30K} = E_c - 0.1$eV
- $\sigma_n^{30K} = 2.3 \cdot 10^{-14}$ cm^2

+/- charged at RT

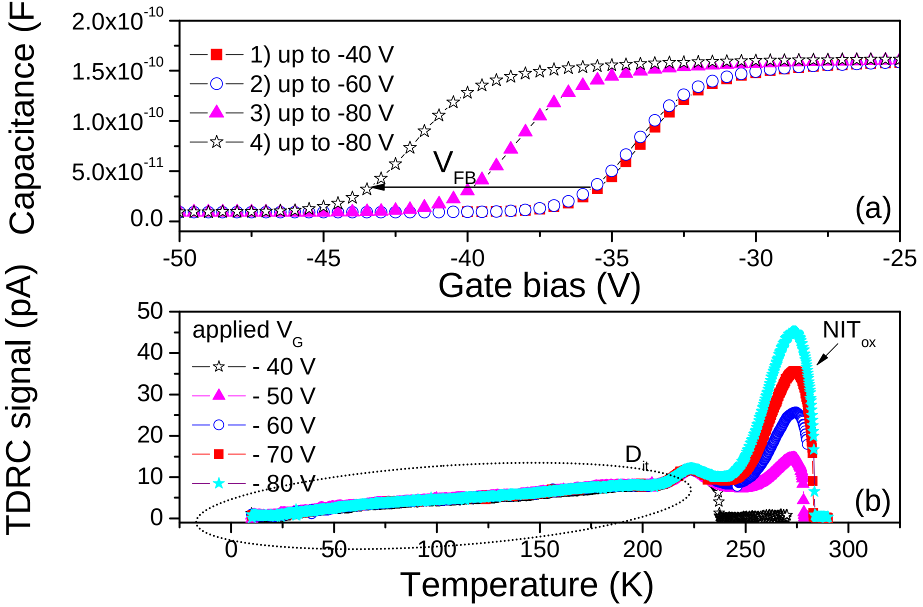


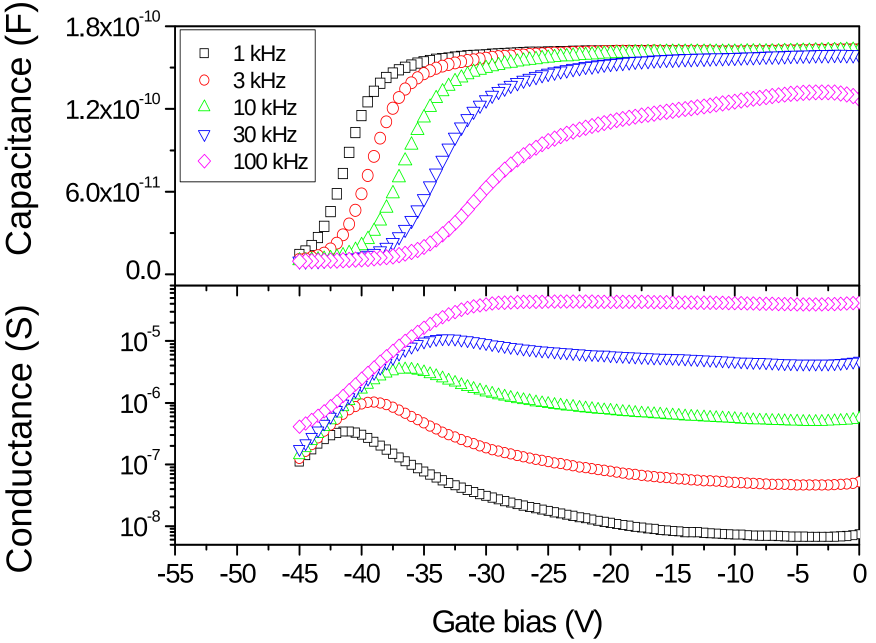
• Surface and interface related effects caused by X-rays in Si based MOS capacitors

- Test structures: MOS (metal-oxide-semiconductor) capacitors fabricated by CiS (http://www.cismst.org/) on 280 μm n-doped <100> and <111> substrates of 5–6 kΩ cm, with the insulator made of 350 nm SiO_2 covered by 50 nm Si_3N_4.
- Irradiations: Irradiation doses from 12 kGy to 1 GGy; X-ray irradiation facility (Perrey, 2011) at DORIS, DESY;
- Measurements: C (f,V), G(f,V), Thermally Dielectric Relaxation Current (TDRC)

Defect states and their impact on electrical properties of the MOS capacitors

10 MGy dose



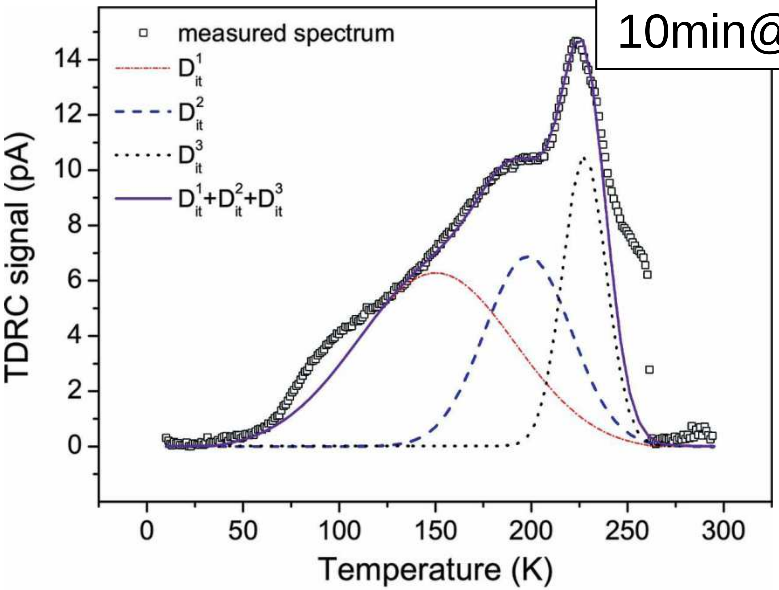


- interface (Dit) → position, shape and frequency dependence of C/G-V
- near-interface-states in oxide (NIT$_{ox}$) → shift the V_{FB} in C-V/G-V characteristics towards more negative bias and causes hysterezis effects
- N_{ox} → influence the V_{FB} ; *it can be accurately determined only from experiments where no charge of NIT$_{ox}$ take place (avoiding biasing in inversion)*

J. INSTRUM., 6, C11013 (2011); J. Synchrotron Rad. (2012). 19, 340–346; J. INSTRUM. 7, C01006 (2012)

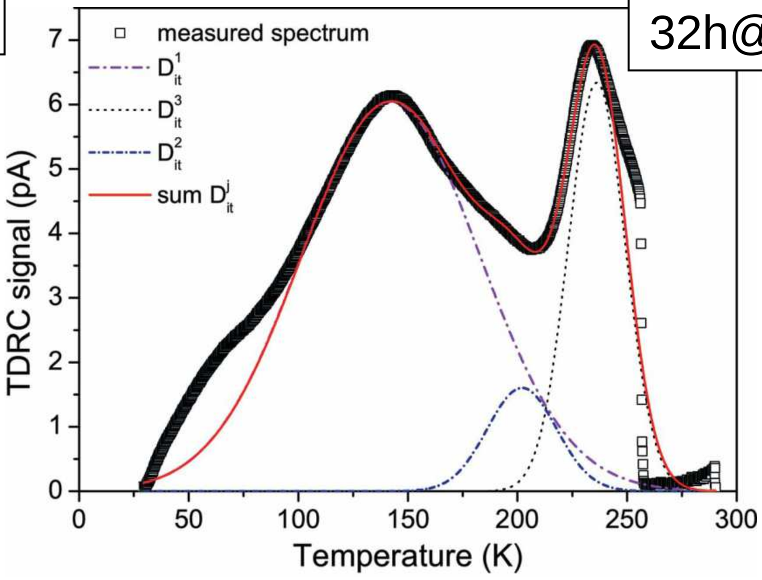
Detection and characterization of Interface states

100 MGy (<100> Silicon)

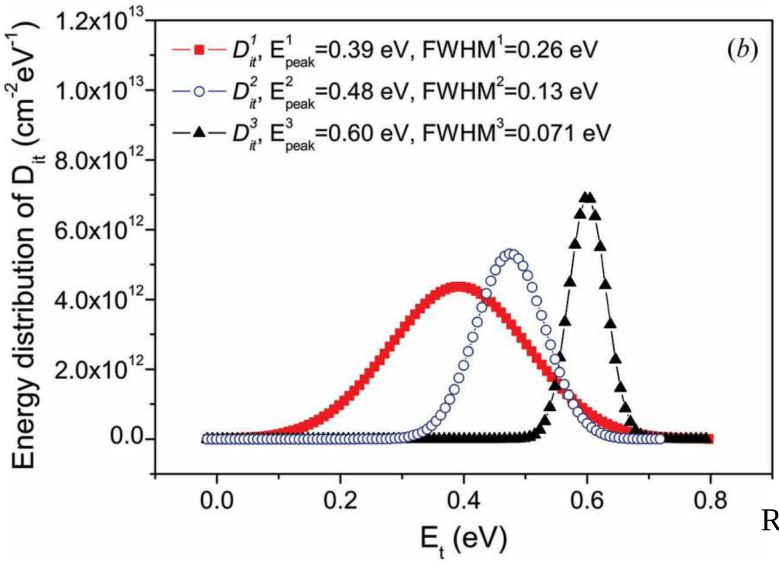


10min@80C

5 MGy (<111> Silicon)



32h@80C

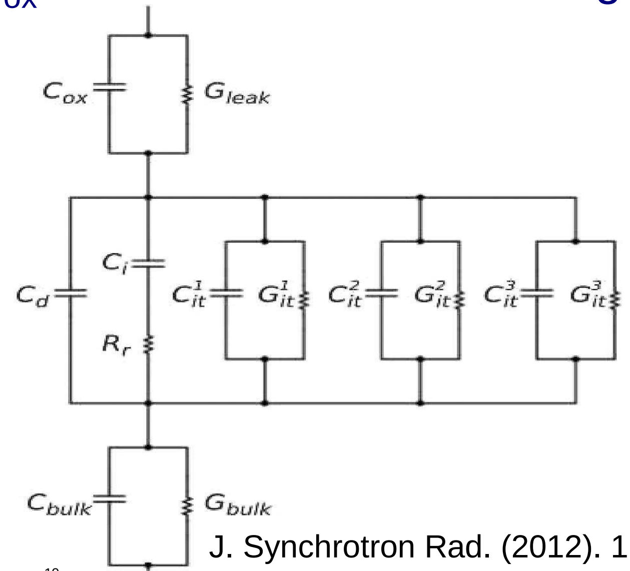


J. Synchrotron Rad. (2012). 19, 340–346

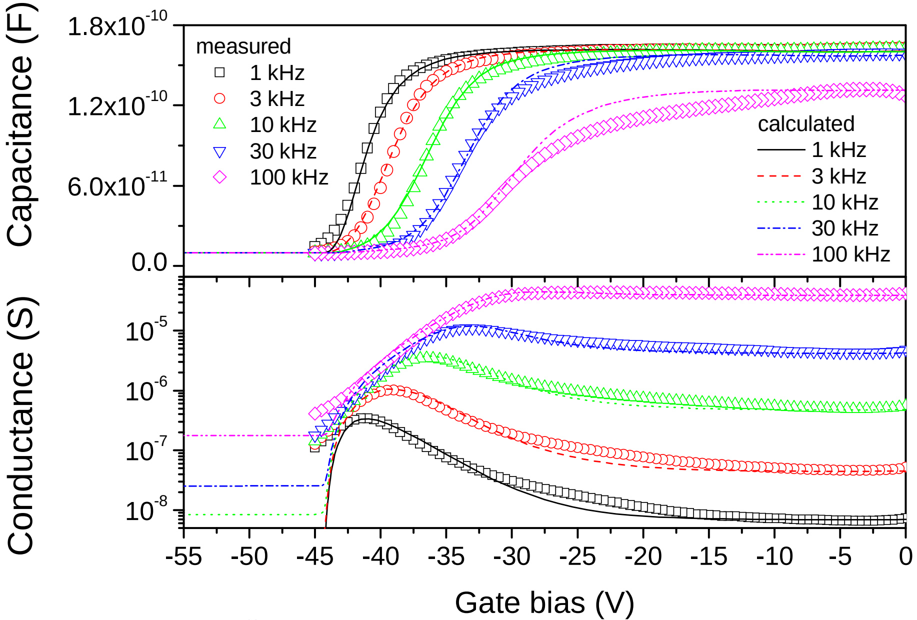
	D_{it}^1	D_{it}^2	D_{it}^3
σ [cm^2]	1.2×10^{-15}	5×10^{-17}	1.0×10^{-15}
peak energy [eV]	0.39	0.48	0.60
FWHM [eV]	0.26	0.13	0.071

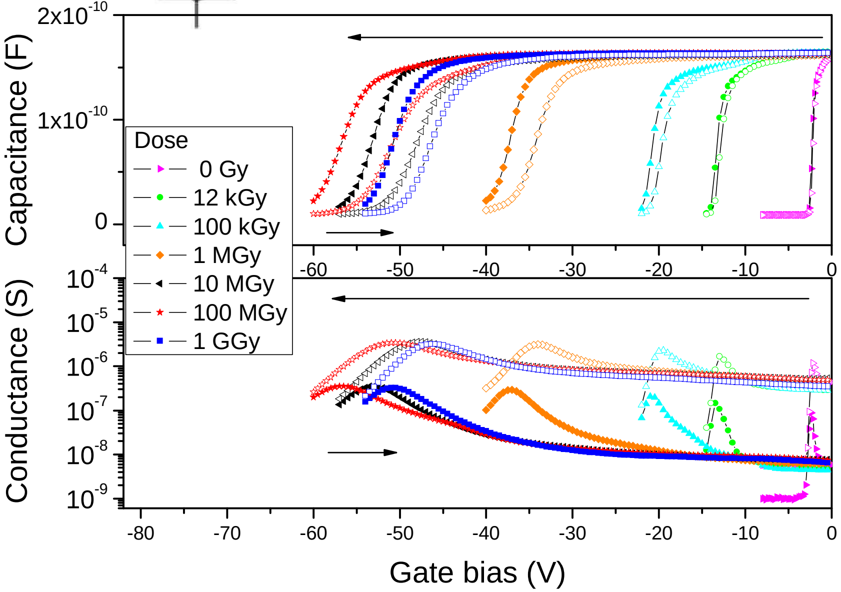
Calculation of C/G-V curves and determination of N_{ox}

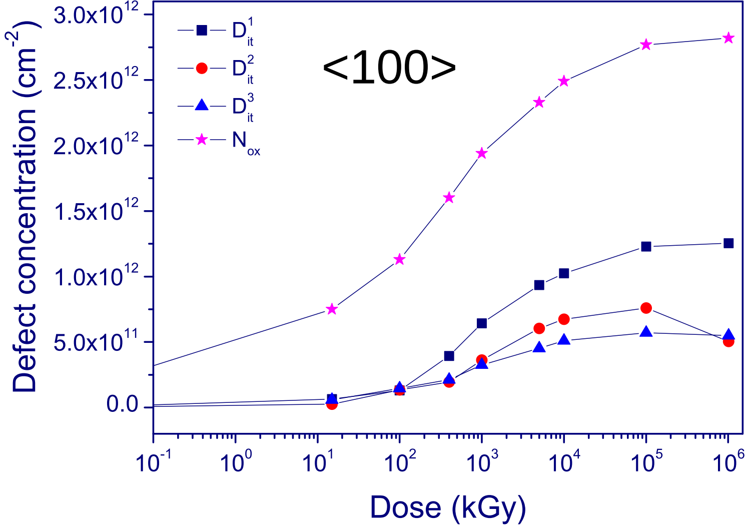
N_{ox} determined from the voltage shift between the measured and the calculated curves



J. Synchrotron Rad. (2012). 19, 340–346







For <111> material the D_{it} and N_{ox} are ~ 20-30 % higher

Conclusions

- Direct correlation between defect investigations and device properties can be achieved! Moreover, when electrical characteristics of the defects are known then models predicting the device performance in different operational scenarious can be developed
- Atomic and electronic point defects – dependent on the material ⇒ defect engineering does work
- Cluster related defects – independent on the material ⇒ Possibility of compensation with point defects via defect engineering
- Still missing the identification of the chemical nature of the defects that deteriorates the device characteristics

Acknowledgements

- University of Hamburg – Inst. for Exp. Physics (Gunnar Lindstroem, Eckhart Fretwurst, Jiaguo Zhang, Gregor Kramberger, Robert Klanner, Joern Schwandt, Hanno Perrey)
- Members of CERN-RD50 Collaboration with special thanks to Michael Moll, Maurice Glasser and Ralf Roeder
- Alexander von Humboldt Foundation