Divacancy-Oxygen Model in Si– fake or fact?

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Evidence for identification of V_2O complex

1976 – the V_2O (**neutral charge state**) was detected by EPR and Photo-EPR studies in CZ Si after heavy electron irradiation (Lee and Corbett)

- ***Induced by irradiation*** – VO+V

  [V_2O] ~ 10% [O] !

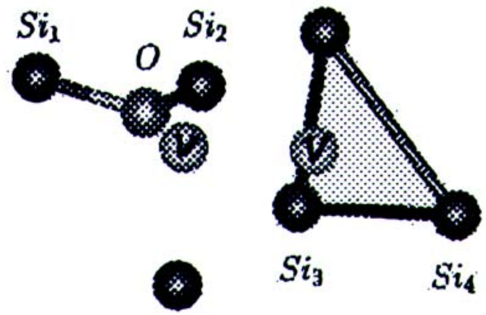
- ***Thermally stable up to 300^o** C in CZ silicon* (up to 25% increase of its concentration during the isochronal annealing up to 300^o C)

- *the increase in its concentration during the heat treatment up to 300^{o}C is believed to be due to (V_2+O) reaction*
- *IR absorbtion – 833.4 cm^{-1} band found to increase upon annihilation of divacancies at 250-300 C and it is atributed to V_2O complex (J.L.Lindström et al, Physica B, 273, 291, 1999)*

- ***Ionization energy*** Ec-0.5±0.05 eV

V_2O formation (theoretical calculations*)

$E_f = 5.5$ eV



1) $V + VO \rightarrow V_2O$

$E_b = 1.4$ eV

2) $VV + O \rightarrow V_2O$

$E_b = 0.5$ eV

⇒ if all V, VV and VO are available (e.g. during irradiation) then reaction 1) is with 0.9 eV more favorable

⇒ reaction 2) has much higher probability to happen (in absence of V) at high temperatures (> 200 C)

***V_2O – two acceptor levels deeper than VO**

****AIMPRO calculations suport three energy levels for V_2O (=/-;-/0,0/+)**

*Pesola et al, PRB 60, 11449, (1999)

** R. Jones – 1st RD50 workshop

V_2O Defect Kinetics Model – as explanation for damage effects (B. C. MacEvoy et al)

V+O →VO first order defect

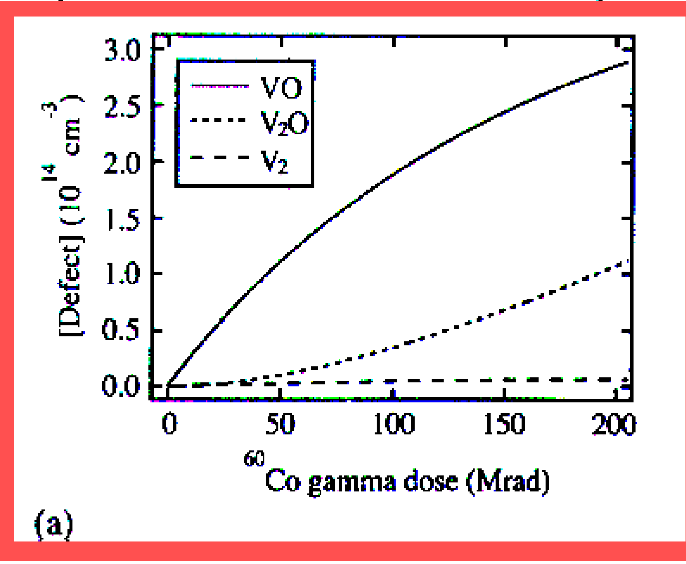
V+VO→ V_2O, second order defect

List A - primary reactions (in the PKA cascade)

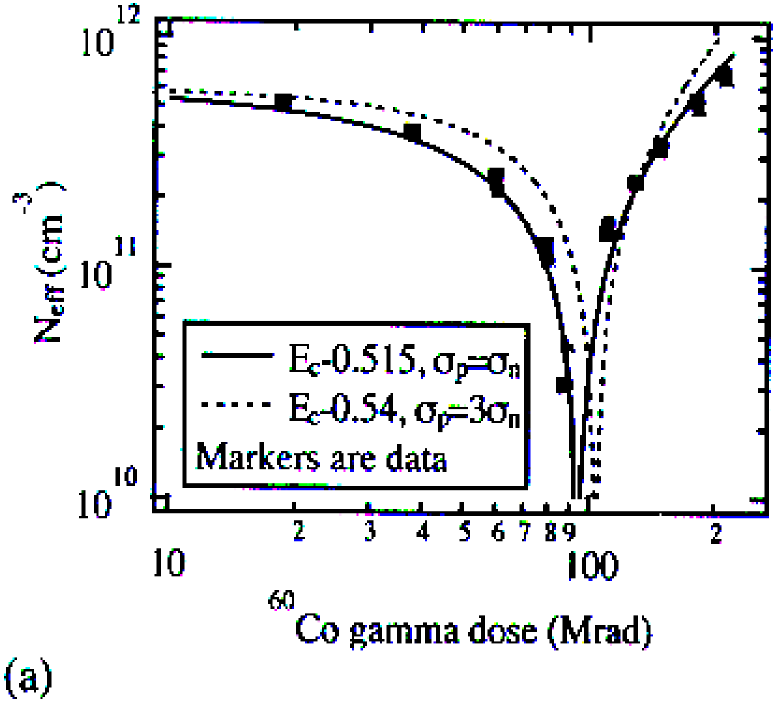
I reactions	V reactions	C_i reactions
$I + V \rightarrow Si$	$V + V \rightarrow V_2$	......

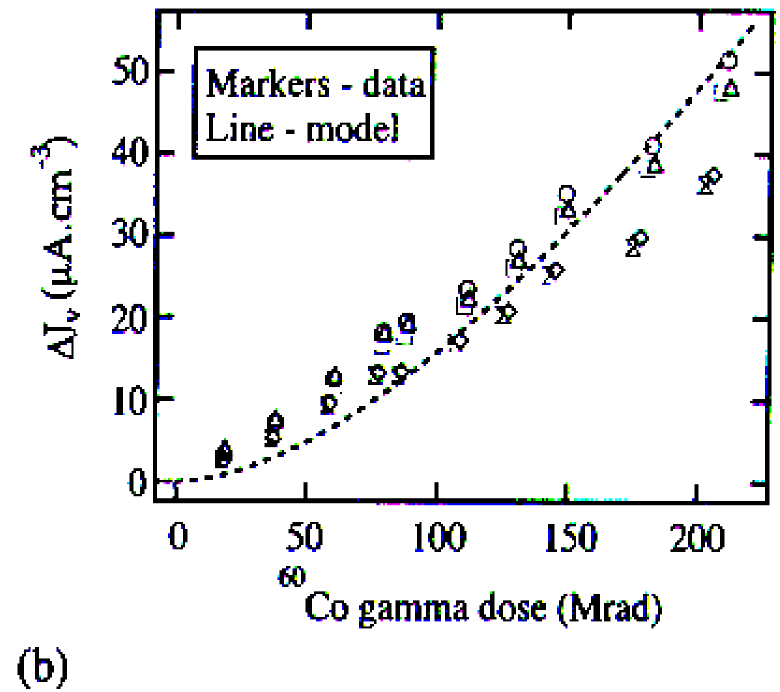
List B - diffusion reactions (outside the cluster)

I reactions	V reactions	C_i reactions
$I + C_s \rightarrow C_i$	$V + V \rightarrow V_2$	$C_i + C_s \rightarrow CC$
	$V + V_2 \rightarrow V_3$	$C_i + O \rightarrow CO$
$I + CC \rightarrow CCI$	$V + O \rightarrow VO$	
$I + CCI \rightarrow CCII$	$V + VO \rightarrow V_2O$	
	$V + P \rightarrow VP$	
$I + CO \rightarrow COI$		
$I + COI \rightarrow COII$		
$I + VO \rightarrow O$		
$I + V_2 \rightarrow V$		
$I + VP \rightarrow P$		



V_2O - Model Predictions





- ***V_2O defect – can be responsable for radiation damage effects***
- ***Beneficial effect of Oxygen enrichment*** - a high [O] would inhibit, via unfavorable competition with the formation of A-center (V-O defect $E_f^* = 3.7$ eV), the formation of V_2O defect ($E_f^* = 5.5$ eV).

- * Pesola et al, PRB 60, 11449, (1999)

Candidates for the V_2O complex

I center* – ***induced by irradiation***

- Amphoteric nature - donor and acceptor states
  $I^{+/0}$ $(E_V+0.23eV)$
  $I^{-/0}$ $(E_C-0.54eV)$
- Quadratic dose dependence u to 400 Mrad
- Evidence for forming via VO center
- Responsable for the damage after γ irradiation
- Thermal stable up to 325^0C **in FZ silicon**

X center** – ***via V_2 annealing in DOFZ silicon***

- Two acceptor like levels
  $X^{=/-}$ - $(E_C$-0. 23 eV),
  $X^{-/0}$ - $(E_C-0.46eV)$
- No data about dose dependence
- Evidence for forming via VV center
- No significant influence to the device properties
- Thermal stable up to 325^oC **in DOFZ**

*I. Pintilie et al, APL 81, 165, (2002), APL 82, 2169, (2003), 2nd RD50 workshop

**E.V. Monachov et al, PRB 65, 233207, (2002), 2nd RD50 workshop

Experimental results

• **Material:**

-Standard float zone (STFZ) and oxygenated (72 h at 1150 C) float-zone (DOFZ)

- Initial doping concentration: STFZ – $8x10^{11}$ cm^{-3}; DOFZ – $1.2x10^{12}cm^{-3}$

- Wacker Si <111> , high resistivity (3-4 kΩcm)

- p^+nn^+ Si diodes, processed by CiS/Erfurt Germany

• **^{60}Co gamma irradiation:**

- Co^{60} γ-source at BNL, dose range 10 to 300 Mrad

• **Measurements:**

• C-V, I-V, at RT

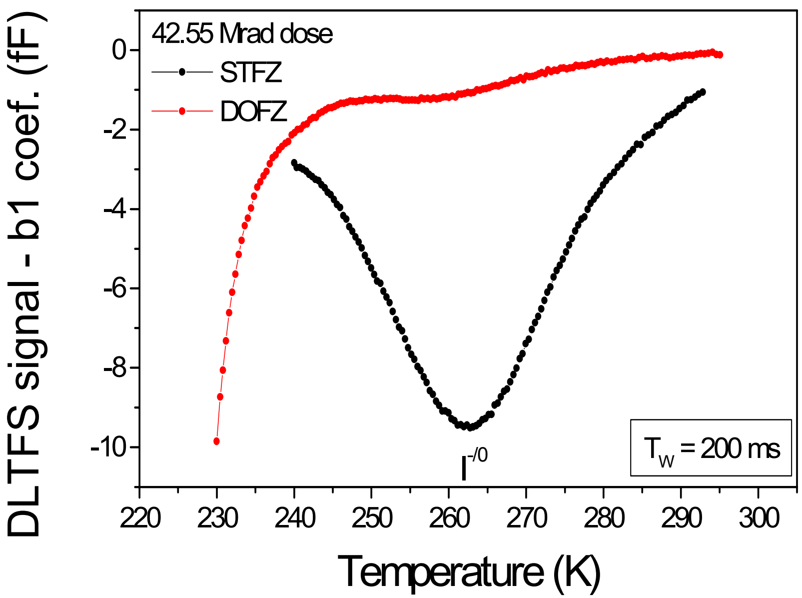
• Deep Level Transient Fourier Spectroscopy – DLTFS

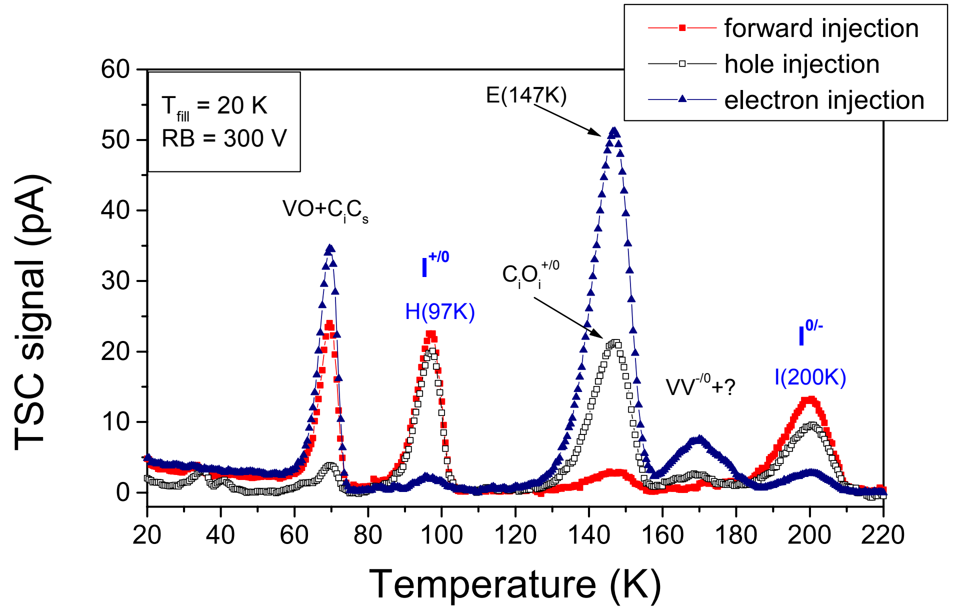
- applied on 4 Mrad irradiated samples

• Thermally Stimulated Current

- applied on high irradiated samples (from 96 to 500 Mrad)

I center





1) Single acceptor state of I center: both -/0 & 0/- transitions (DLTS&TSC)

$I^{-/0}$: $E_a = E_c - 0.545$ eV, $\sigma_n = (1\text{-}3)\times10^{-15}$ cm^2 **$I^{0/-}$**: $E_a = E_v + 0.58$ eV, $\sigma_p = (8\text{-}10)\times10^{-14}$ cm^2

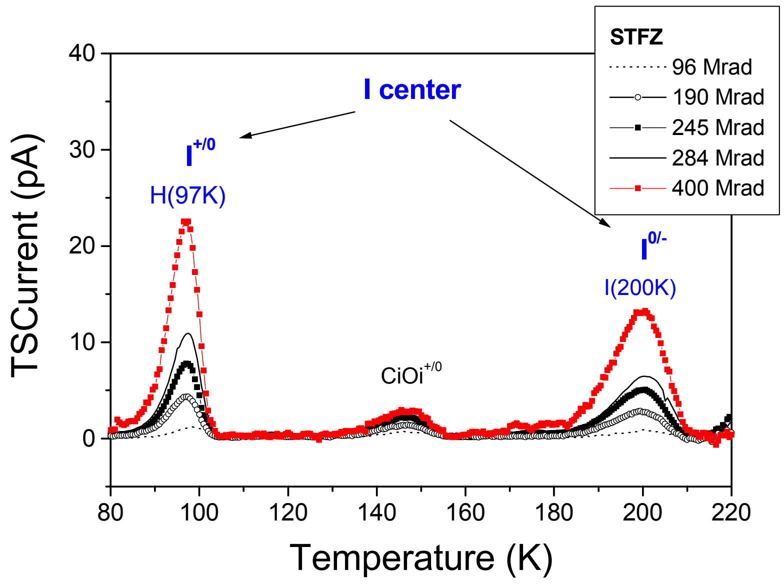
Due to its steady state occupancy

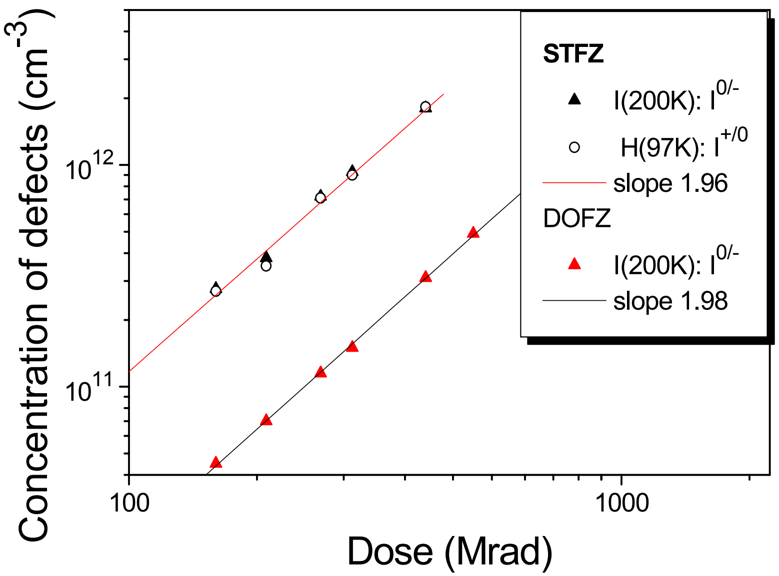
<15% [I] can be detected through e-emission >85% [I] can be detected through h-emission

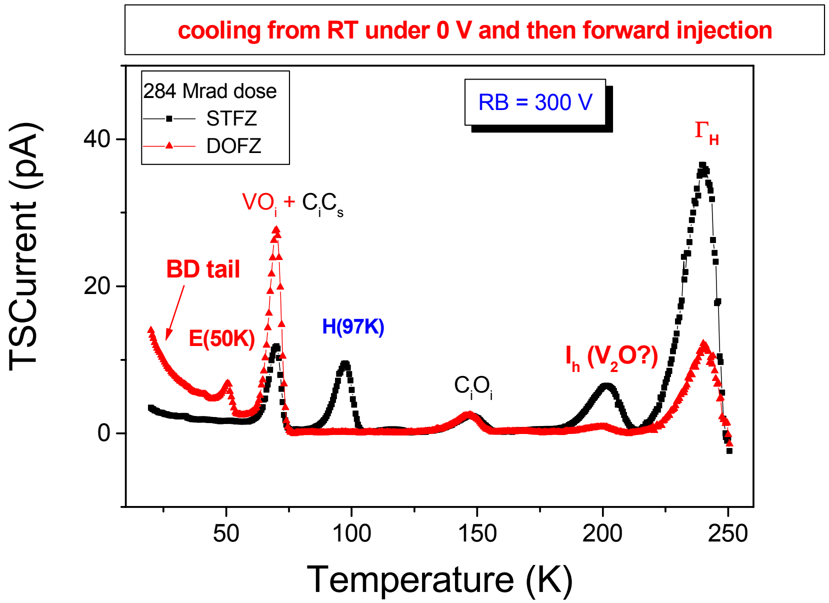
2) **Donor state of I center:** +/0 transition

$I^{+/0}$: $E_a = E_v + 0.23$ eV($\pm$0.01), $\sigma_p = (0.9\text{-}3)\times10^{-14}$cm^2

I center – dose dependence

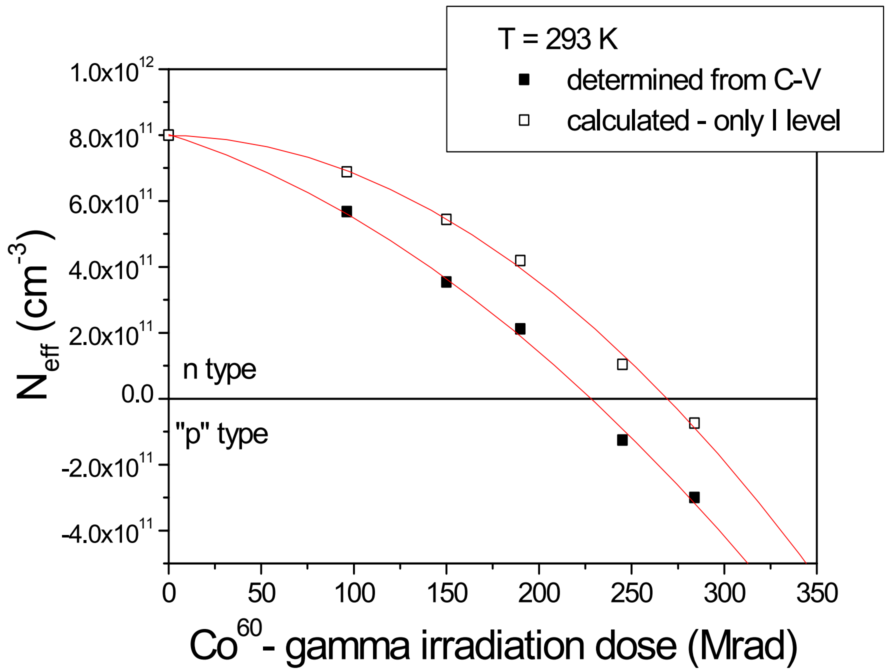


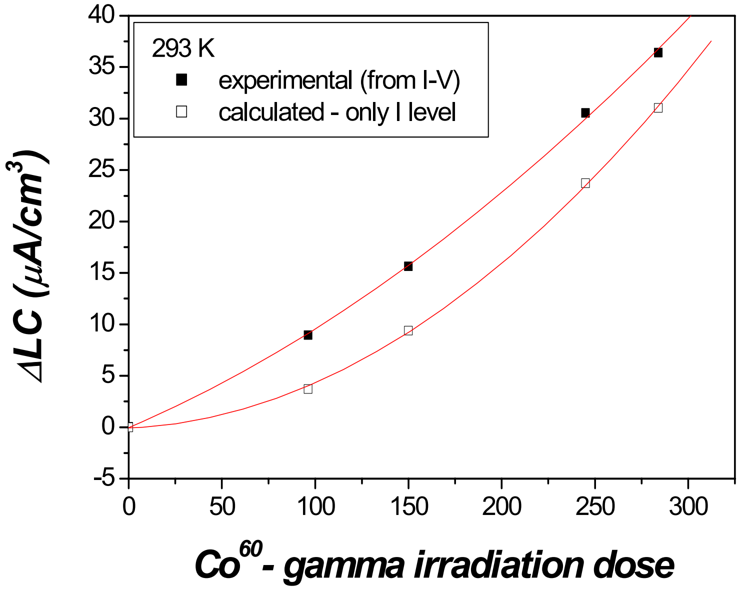




- ***Almost quadratic dose depence***
⇒ evidence for formation via two primary induced defects (one is VO)
- ***Largely suppressed in oxygen rich material***

I center
& device performance



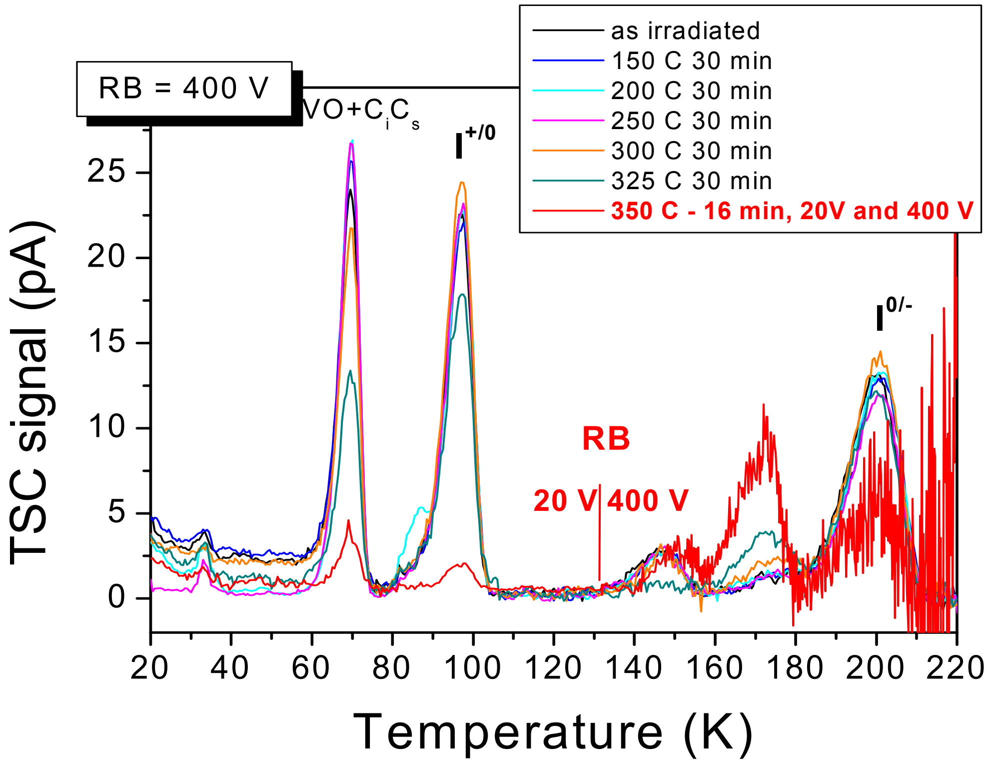


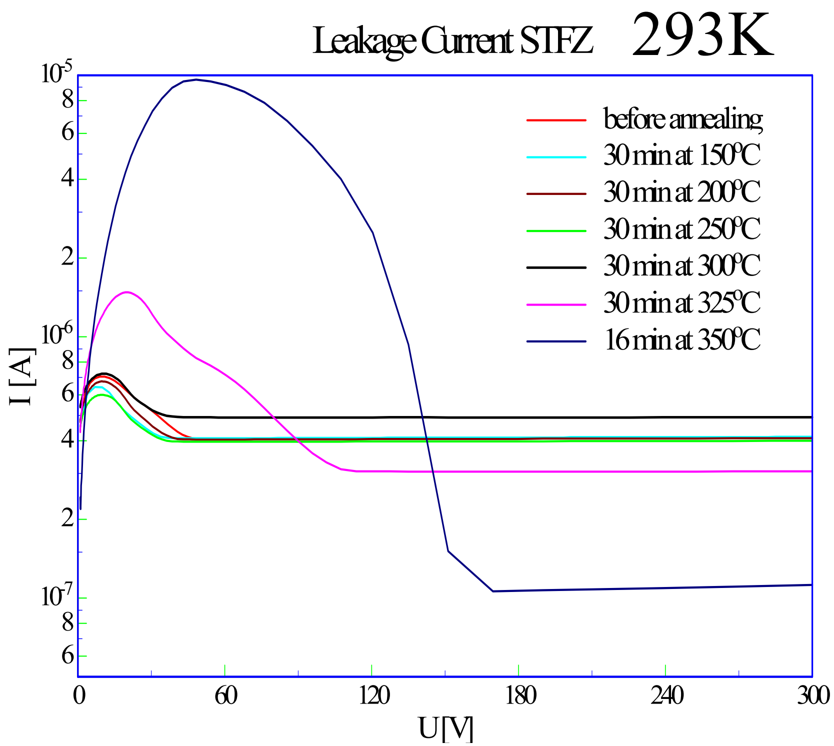
I center - responsable for:

- ***type inversion in STFZ material***
- ***increase of the leakage current in both STFZ&DOFZ silicon***

I center – thermal stability

Isochronal annealing

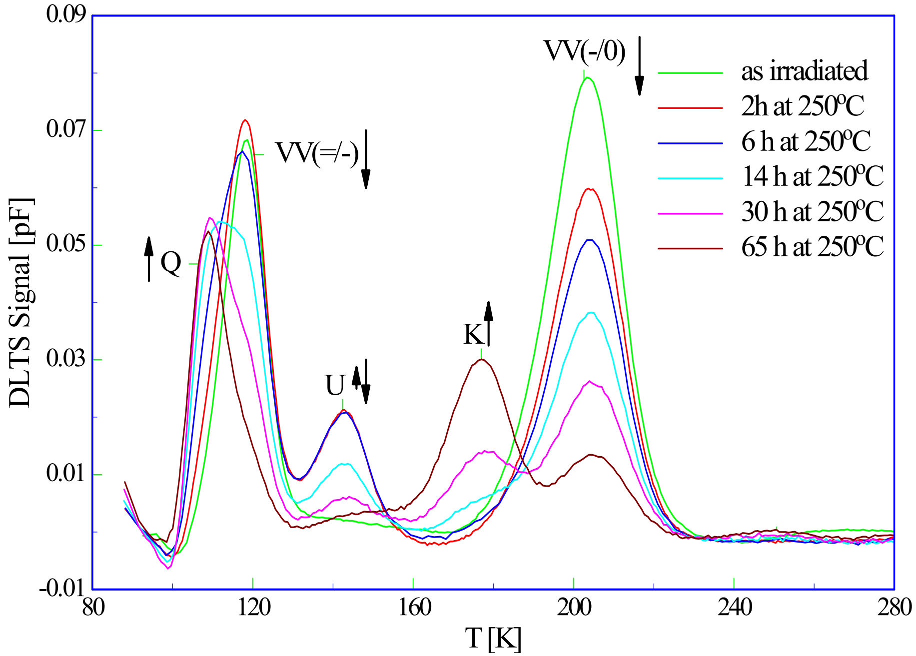




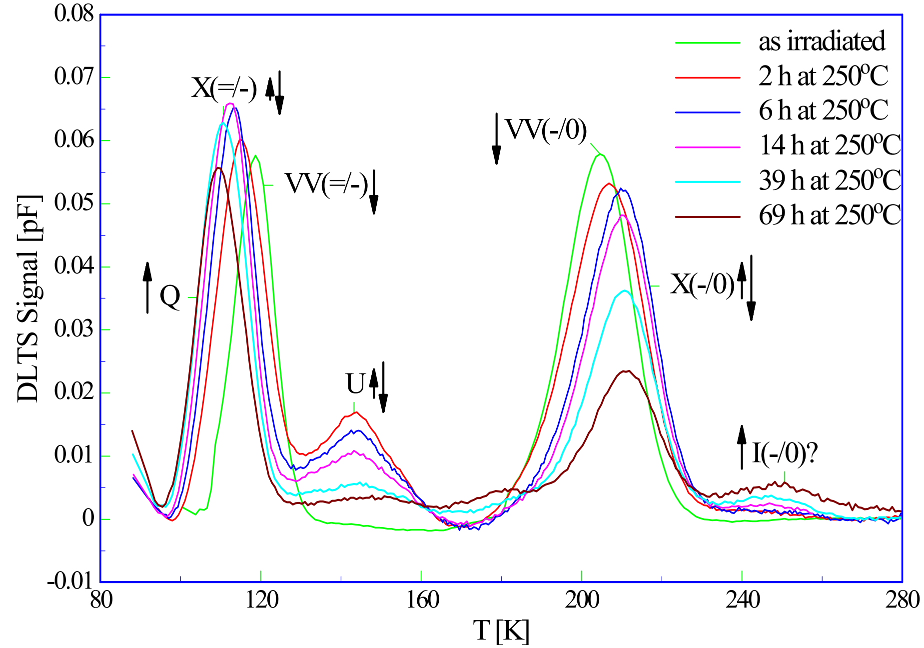
Stable up to 325 °C

X center – formed in DOFZ silicon during 250°C annealing

STFZ: VV ↓ – ↑ Q&U&K



DOFZ: VV ↓ – ↑ U&X&Q



Q: E_a = 0.21 eV; $\sigma_n^a = 2x10^{-15}$ cm^2

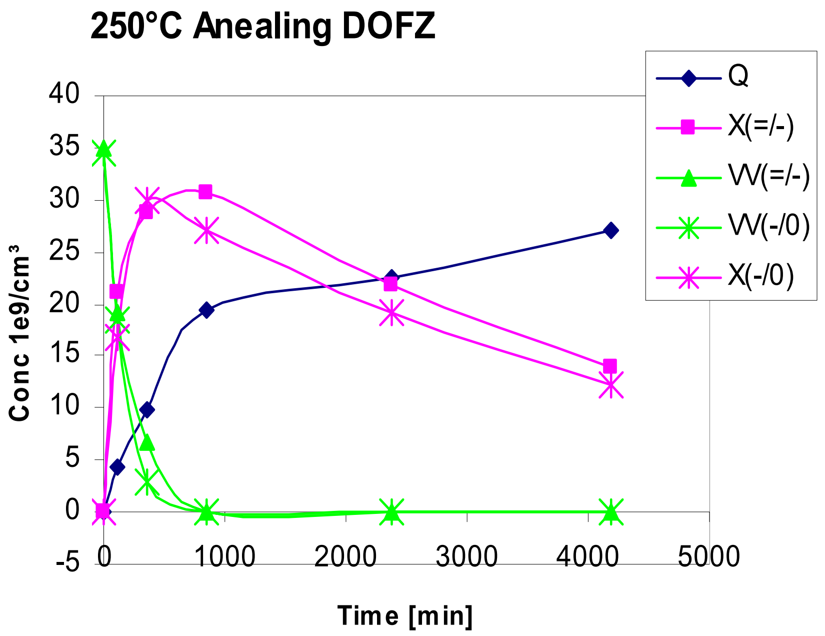
U: E_a = 0.3 eV; $\sigma_n = 7x10^{-15}$ cm^2

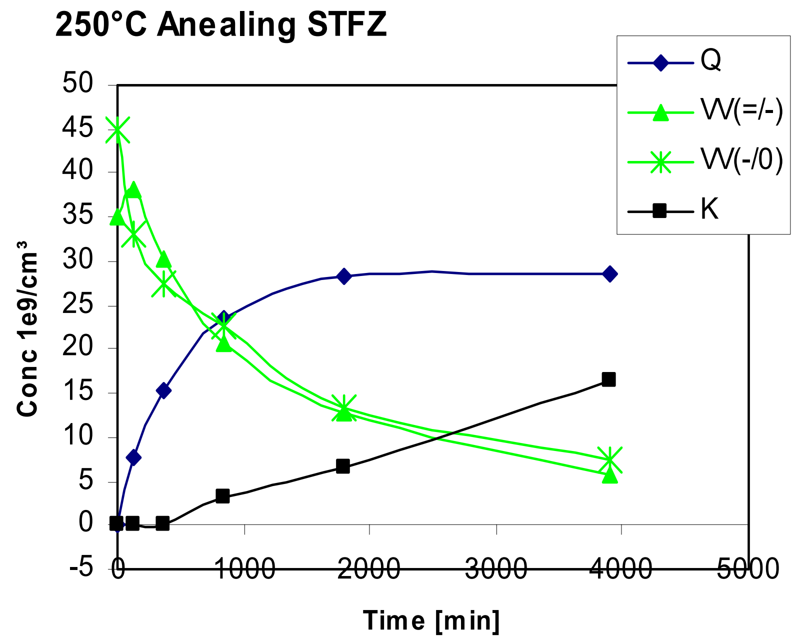
K: E_a = 0.31 eV; $\sigma_n = 8x10^{-17}$ cm^2

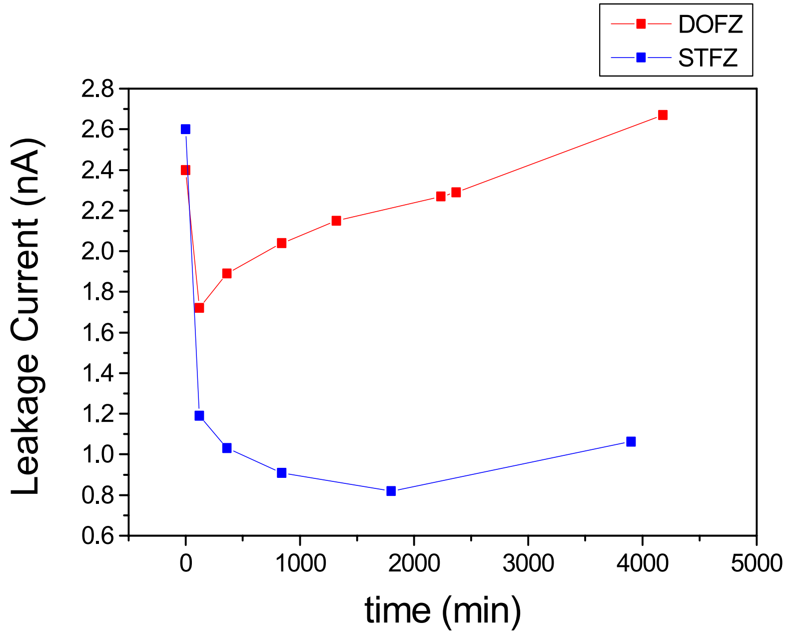
$X^{-/0}$: E_a = 0.465 eV; $\sigma_n = 1.1x10^{-14}$ cm^2

$X^{=/-}$: E_a = 0.23 eV; $\sigma_n = 1x10^{-16}$ cm^2

When X starts to anneal out a deeper level (possible I center) starts to form





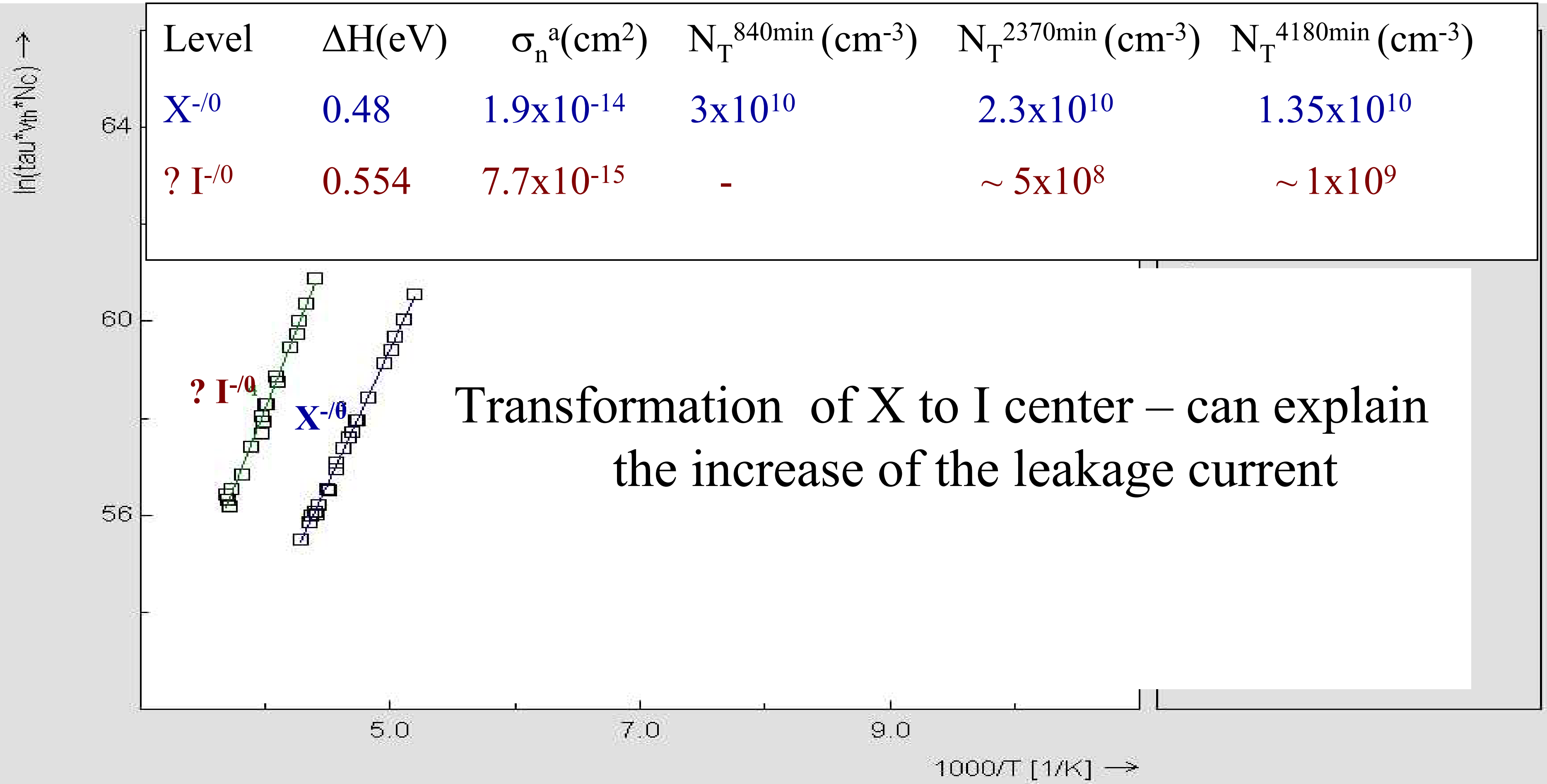


The leakage current in DOFZ continue to increase also after X centers start to anneal out

$\Rightarrow$ Deeper centers form

Annealing of X center – forming of I complex ?

Level	ΔH(eV)	σ_n^a(cm^2)	N_T^{840min} (cm^{-3})	$N_T^{2370min}$ (cm^{-3})	$N_T^{4180min}$ (cm^{-3})
$X^{-/0}$	0.48	1.9×10^{-14}	3×10^{10}	2.3×10^{10}	1.35×10^{10}
? $I^{-/0}$	0.554	7.7×10^{-15}	-	$\sim 5 \times 10^{8}$	$\sim 1 \times 10^{9}$



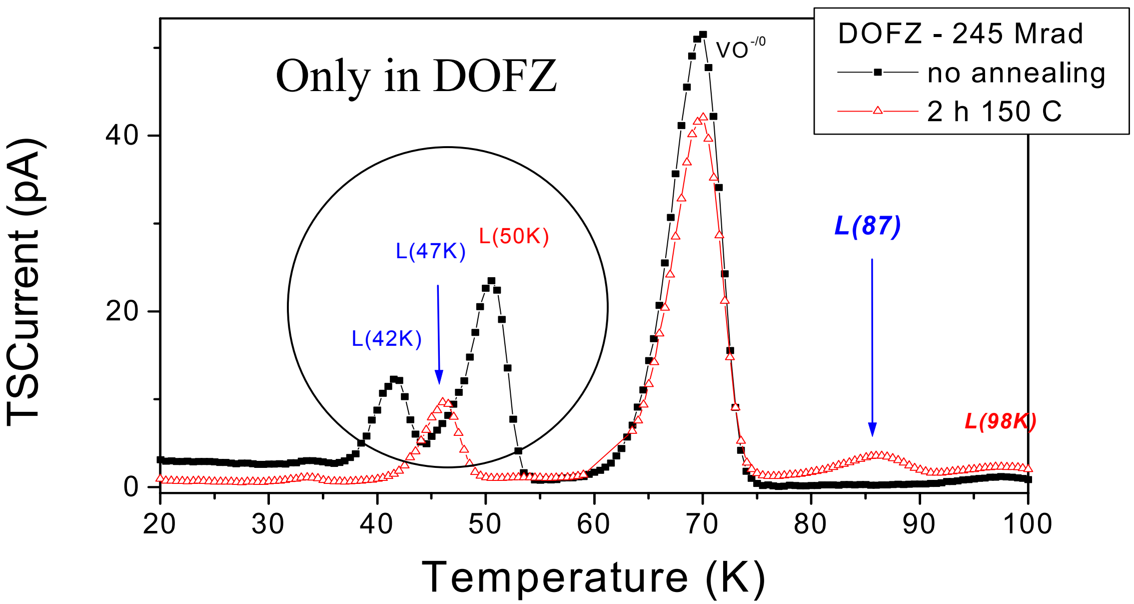
Transformation of X to I center – can explain the increase of the leakage current

Close to some conclusions

- ***I & X centers – both are oxygen related and stable up to 325º C***
- ***During X annealing – I may form***
- X center: fomed in oxygen rich material via VV annealing – is it another configuration of VV prior to form V_2O, V_2O or V_2O_2 ? – in any case will not explain the observed damage effects

Considering also the changes in the concentration of oxygen related much shallower levels ⇒ oxyen dimers might be involved in formation of X centers

Annealing of L(42K) and L(50K) - ***posible IO_2 complex***
L(87)(hole trap formed after annealing of L(42K)&L(50K)



- IR absorbtion data*

$IO_2 \rightarrow I+O_{2i}$ at ~150º C

*J.L.Lindstöm et all,Nucl. Instr.& Methods B, 186, 121, 2002

- $O_{2i}+VV \rightarrow V_2O_2$

• ***I center*: second order defect formed via VO – is it V_2O or V_2O_2?**

1) I: $V+VO \Rightarrow V_2O$

2) $V+O_2 \Rightarrow VO_2$

$V+VO_2 \Rightarrow V_2O_2$

V_2O should form in higher concentration than V_2O_2 (higher V′ introduction rate and lower binding energy)

Conclusions

• ***Most likely* I center is V_2O and X center is another VV configuration or V_2O_2 $\Rightarrow$ experimental confirmation the V_2O model!**

• ***Less probable* (but not impossible) – X is V_2O and I center is V_2O_2 $\Rightarrow$ the „V_2O model“ should change to „V_2O_2 model“**