# Can cluster physics shed some light on the puzzles of our Experimental findings with energetic particles?

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## Introduction

Leakage current /
Carrier removal / ???clusters???
Annealing /

## 1. Cluster formation

(Vinetskii and Kondrachuk in Rad. Effects 1975, vol.30 p227)

first stage: high-energy particles displace matrix atoms
point defects: vacancies(V), interstitials(I)

second stage: diffusion of vacancies and interstitials
quasimolecules (secondary radiation defects)

Model for second stage:

Mobility of I>>V

2 reactions V+V → D reaction constants
V+O → A $\alpha_D$, $\alpha_A$

Diffusion equation for vacancies and reaction equation for Oxygen and initial conditions at center of cluster $N_o$

system of nonlinear equations

dimensionless parameter

$$\varepsilon = \frac{D_V}{\alpha_D N_0 L^2}$$

L characteristic size of cluster

N and L depend on incident particle, while ~~and~~ $D_V$, $\alpha_D$
Depend on crystal properties

a) $\varepsilon$ <<1 low vacancy diffusion → congealing cluster
shape of D-cluster ~ V-cluster (original)

b) $\varepsilon$ >>1 high vacancy diffusion → spreading cluster

belt of A centers around D-cluster
energy threshold of knock-on atom between 2 cases 10keV

## 2.Properties of cluster

2.1 structure → central region (core): vacancies + interstitial associations
→ peripheral region (impurity defect shell)
bell shape of distribution

2.2 electrical field center: charged D depending on Fermi level
periphery: charged impurity defects
local charge neutrality: (acceptors, donors, free carriers)

Poisson equation + charge neutrality → selfconsistent system which yields occupation probability of acceptors $f_i$ and potential barrier $\Psi_0$ between matrix and center of cluster
Approximate solution of Poisson equation

$$\Psi_0 \approx \frac{2\pi e^2 r^2}{\epsilon} \sum_i N_i f_i - \frac{kT}{3}$$

$$f_i = \frac{1}{1 + N_c/n_g \exp\left[-\frac{\Psi_0 - \Delta E_i}{kT}\right]}$$

where r is radius of cluster and $\Delta E_i$ energy position of defect in forbidden bandgap
$N_i$ density of defect

## 2.3 Parameter description

**Kuznetsov and Lugakov, phys.stat.sol(a) vol.79, p381 (1983)**
**Temperature dependencies of Hall coefficient + nature of defect**

Defect cluster parameters in n-Si

| irradiation | material | $n_0$ ($10^{13}$ cm$^{-3}$) | core $\psi$ (eV) | core radius (Å) | core radiation defect density (cm$^{-3}$) | periphery $\psi$ (eV) | periphery radius (Å) | periphery radiation defect density (cm$^{-3}$) |
|---|---|---|---|---|---|---|---|---|
| neutrons | float-zone | 3 | ≈0.14 | ≈ 130 | $\approx 8 \times 10^{17}$ | ≈0.03 | ≈ 600 | $\approx 1.7 \times 10^{16}$ |
| neutrons | pulled | 2 | ≈0.14 | ≈ 130 | $\approx 8 \times 10^{17}$ | 0.05 | 300 | $1.2 \times 10^{17}$ |
| protrons | float-zone | 1 | 0.11 | 1800 | $7 \times 10^{15}$ | 0.02 | 15000 | $2.7 \times 10^{13}$ |
| protons | float-zone | 3 | 0.11 | 1800 | $7 \times 10^{15}$ | 0.023 | 13000 | $4.3 \times 10^{13}$ |
| protons | float-zone | 8 | 0.11 | 1800 | $7 \times 10^{15}$ | 0.025 | 12000 | $5.8 \times 10^{13}$ |
| protons | float-zone | 1.6 | 0.11 | 1800 | $7 \times 10^{15}$ | 0.03 | 9000 | $1.6 \times 10^{14}$ |
| protons | pulled | 2 | 0.11 | 1800 | $7 \times 10^{15}$ | 0.03 | 6000 | $2.8 \times 10^{14}$ |
| protons | pulled | 5 | 0.11 | 1800 | $7 \times 10^{15}$ | 0.033 | 6000 | $2.8 \times 10^{14}$ |
| protons | pulled | 30 | 0.11 | 1800 | $7 \times 10^{15}$ | 0.04 | 5000 | $5.3 \times 10^{14}$ |

## 2.4 Strain field

| | |
|---|---|
| **Deposited energy** | **~10000 eV in** |
| **a cluster volume** | **~10 E-18 cm-3** |
| **Temperatur diff** | **~1000 K** |
| **Fast cooling in** | **~10E-10 s** |
| **Pressure** | **~10000 bar** |

## 2.5 Divacancy levels in cluster

**A.V. Vasil'ev et al. Sov.Phys.Semicond. vol.20(4) p465 (1986)**

**For locally inhomogeneous distribution of deep levels**

$$N_d^- = N_T M \int_V F(r) f(T, E_F - E_d)\, dV$$

where $\int_V F(r)\, dV = 1$

and $f(T, E_F - E_d)$ - occupancy

$N_d^-$ Volume average concentration of charged center

$N_r$ Concentration of local region

Analysis performed with following assumptions

- homogeneous distribution of D in matrix +embedded local regions with M divacancies in it.
- bell shape of initial cluster

$$F(r) = \frac{1}{\pi^{3/2} L^3} \exp(-r^2/L^2)$$

- only divacancy level $E_c$ -0.39 eV considered
- N depends linearly on dose

A. V. Vasilev et al.
Sov. Phys. Semicond.
20 p 465 (1986)

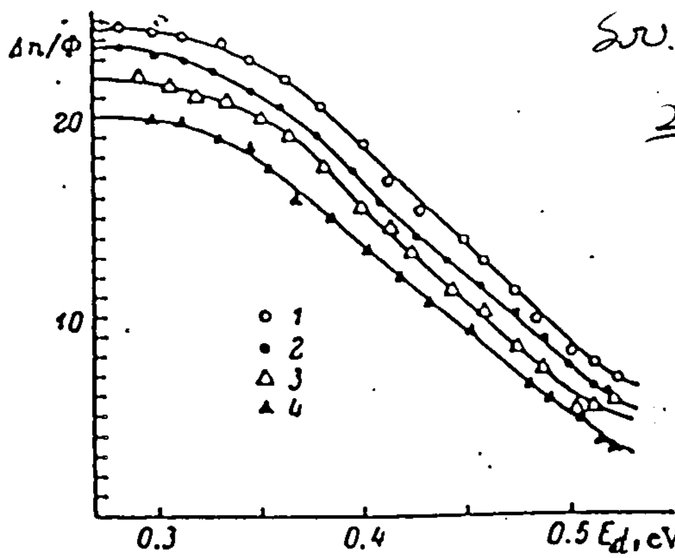



FIG. 1. Values of Δn/Φ obtained at temperatures 250–450 K for zone-grown (1) and crucible-grown (2-4) samples. Radiation dose Φ ($10^{12}$ $cm^{-2}$): 1), 2) 0.5; 3) 1.0; 4) 1.5. The experimental points were taken from Ref. 7. The continuous curves are theoretical dependences calculated on the assumption of a locally inhomogeneous distribution of divacancies in a crystal (Table II). $n_0 = 5 \cdot 10^{13}$

α at 6.3 MeV  no $V^=$ state !!

## 3. Consequences for ROSE problems

### 3.1 Carrier Recombination

Most likely recombination centers are D

Problem of capture coefficient for free carriers

If there is a potential barrier built-up inside cluster:

Holes attracted into interior

Electrons pushed to matrix depletion

Then effective capture cross section for holes

$$\sigma_p^* = \sigma_p \exp\left(\frac{\psi}{kT}\right) \cdot K_s$$

$K_s$ is a factor for fact that potential barrier $\psi$ is not abrupt but extends to a Debeye screening length for the case that this length is smaller than outer cluster radius

$K_s$~vol of total cluster / volume of negativ charge

For $n_0 \geq 3 \cdot 10^{13}\ cm^{-3}$ $K_s \exp\left(\frac{\psi}{kT}\right) \sim 30$

P.F.Lugakov and V.V.Shusha Rad. Effects vol.62 p197 (1982) and Stefanov et al. Phys.stat. sol.(a) vol 163 p27 (1997) find

$\sigma_p/\sigma_n \approx 150$ for clusters

and $\sigma_p/\sigma_n \approx 22$ electron irradiated Si

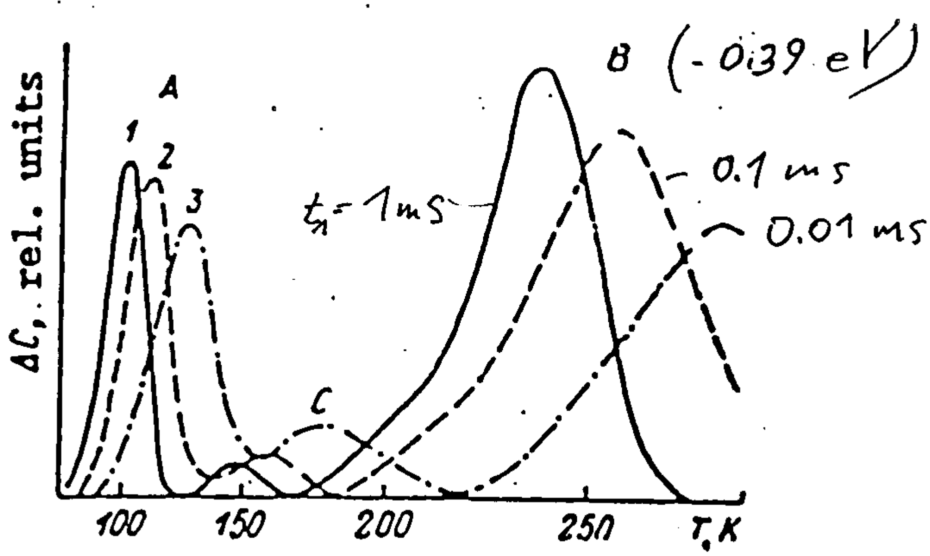
This yields $K_s \exp(\psi/kT) \sim 7$ for 2kOhmcm Si

M.Moll needs 6

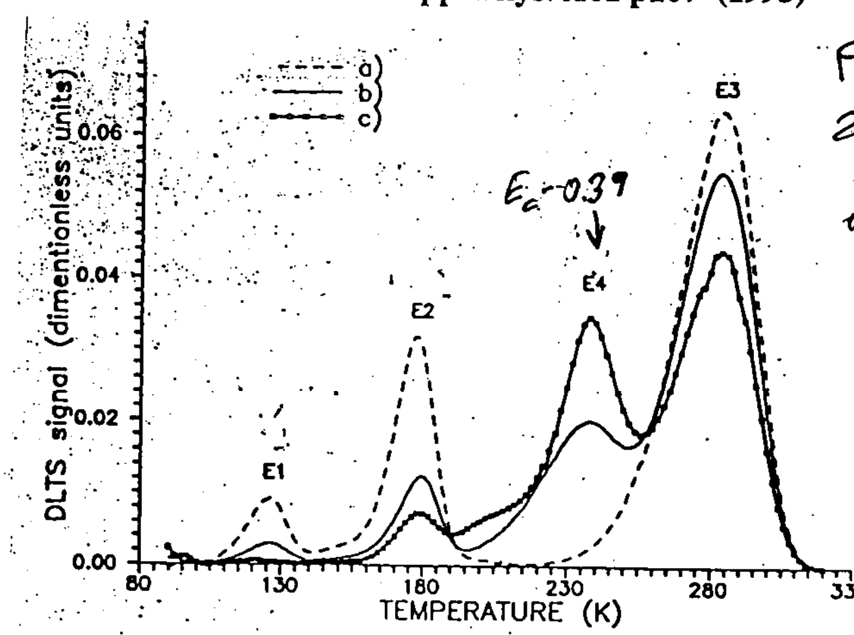
### 3.2 DLTS measurements

**Careful with interpretation, since charging of traps in potential well of clusters not guaranteed**
**Capture rate of carriers >> thermal release of carriers**
**I.V. Antonova et al. Sov.Phys.Semicond. vol.22(6) p630 (1988)**
**Broadening + temperature shift of E peak**

reactor neutrons




**and Ch.M.Hardalov et al. Appl.Phys. A61 p107 (1995)**




$p^+ n n^+$
2000 Ωcm
↓
detector grade
4.5 MeV
neutrons

**Fig. 1.** DLTS spectra of non-irradiated sample (*a*); irradiated with a fluence of $5.5 \times 10^{11}$ n/cm$^2$ (*b*); and with a fluence of $1.0 \times 10^{12}$ n/cm$^2$ (*c*)

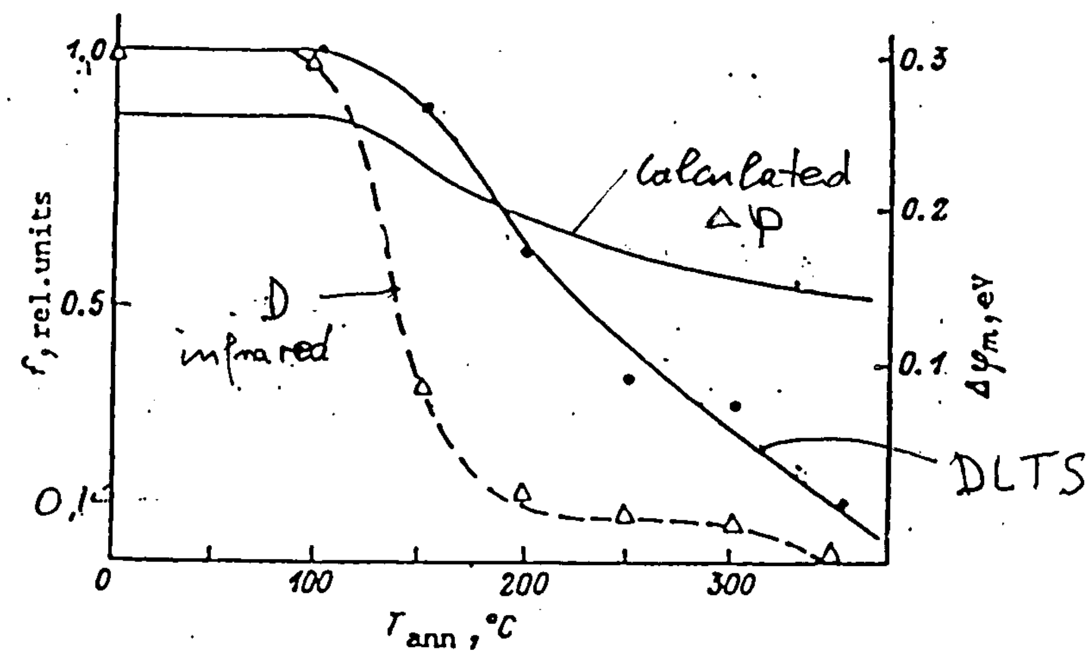
| | E1 | E2 | E3 | E4 | $\sigma_e$ cm$^2$ |
|---|---|---|---|---|---|
| Before radiation | 0.21 | 0.31 | 0.49 | | |
| After 5.5 10 E11 | | | | 0.43 | 2.E-15 |
| After 10 E12 | | | | 0.33 | 2.E-17 |

Extend of cluster space charge layer (CSCL) ~ 3 microns
Debeye length

Overlap of CSCL after a fluence 10E12 cm-2
Fabrication defects (shallow) masked by local potential

## 3.3 Annealing of D in Si containing clusters

3.31 I.V.Antonova et al. Sov.Phys.Semicond. vol .23 p671 (1989)




CZ $n_t$ 3.5 $10^{15}$
$\Phi$ 4.4 $10^{-14}$ cm$^{-2}$

D = 95
$R_0$ = 220 Å

observation: anneal in 2 stages

250 - 350°C classical $E_a$=1.5eV

100 - 200°C smooth / different mechanisme

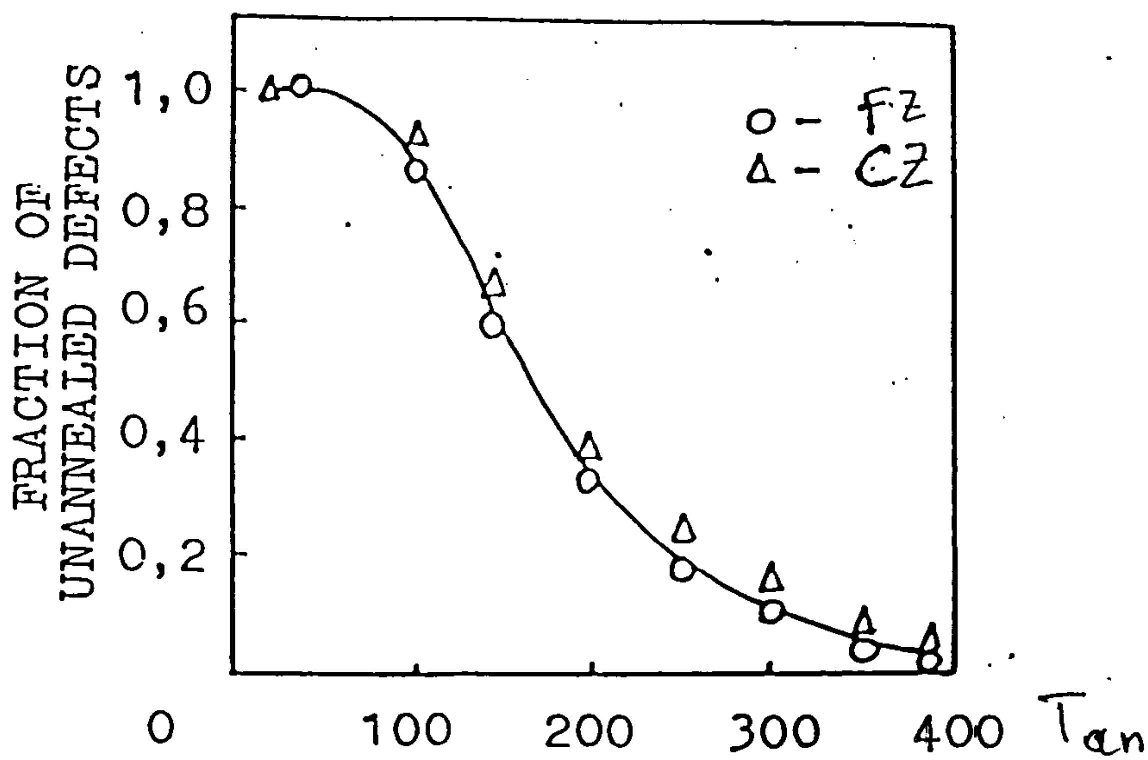
at 120°C $I_2 \longrightarrow I + I$

$I + C_s \longrightarrow C_i$

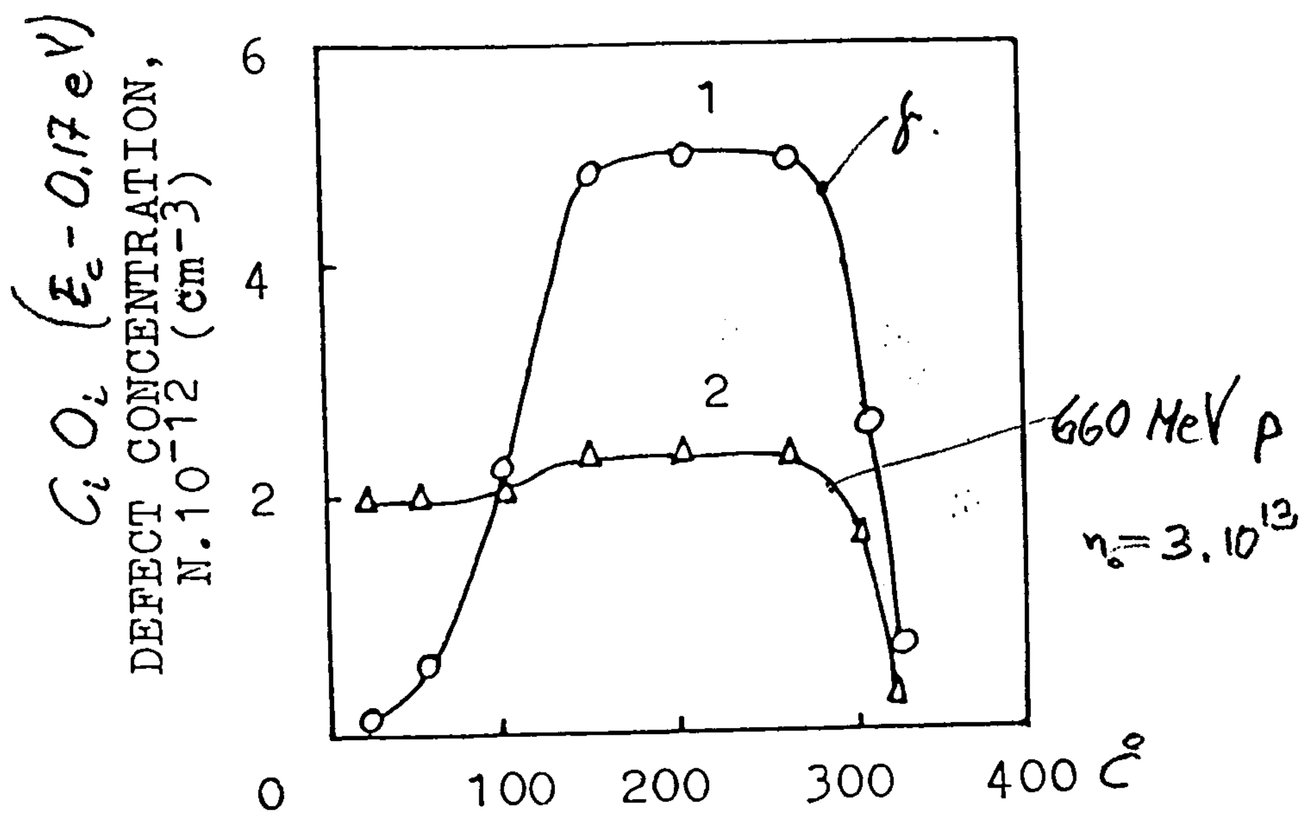
$C_i \longrightarrow$ cluster (strain)

### 3.31 Peculiar observations

V.I. Kuznetsov et al. Rad. Effects Lett. Vol.86 p199 (1984)




$n_o = 3 \cdot 10^{13}$ 660 MeV prot.

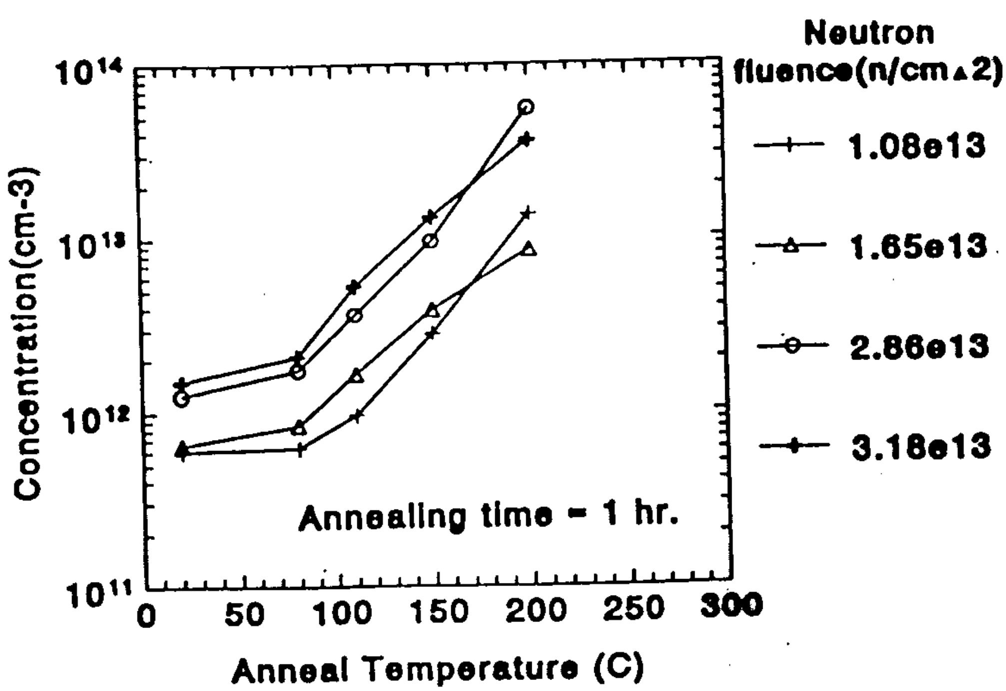



**Indirect proof of $C_i$ annealing: more than 2 times of $C_i$ goes into cluster**

**Effect of strain field: $C_i$ cause lattice compression**
**D cause lattice tension**

### 3.3 Annealing of ROSE detectors

**Z.Li et al. NIM A 385 p321 (1997)**



## 4. Model for positive and negative annealing

**Be cautious!! Might be crab!!**

**Suppose: main defect D distributed as point defects in matrix**
**or forming a cluster**
**potential barriers and strain field around cluster**

**irradiation produces Interstitials which go to sinks**

Sinks:

$$\begin{cases} I + C_s \longrightarrow C_i \\ I + OV \longrightarrow O_i \\ I + V_2 \longrightarrow V \\ I + P_s \longrightarrow P_i \end{cases}$$

**$C_i$ are mobile and get eventually settled in**

Sinks:
- $C_iC_s$
- $C_iO_i$
- D in cluster
- D in matrix (?)

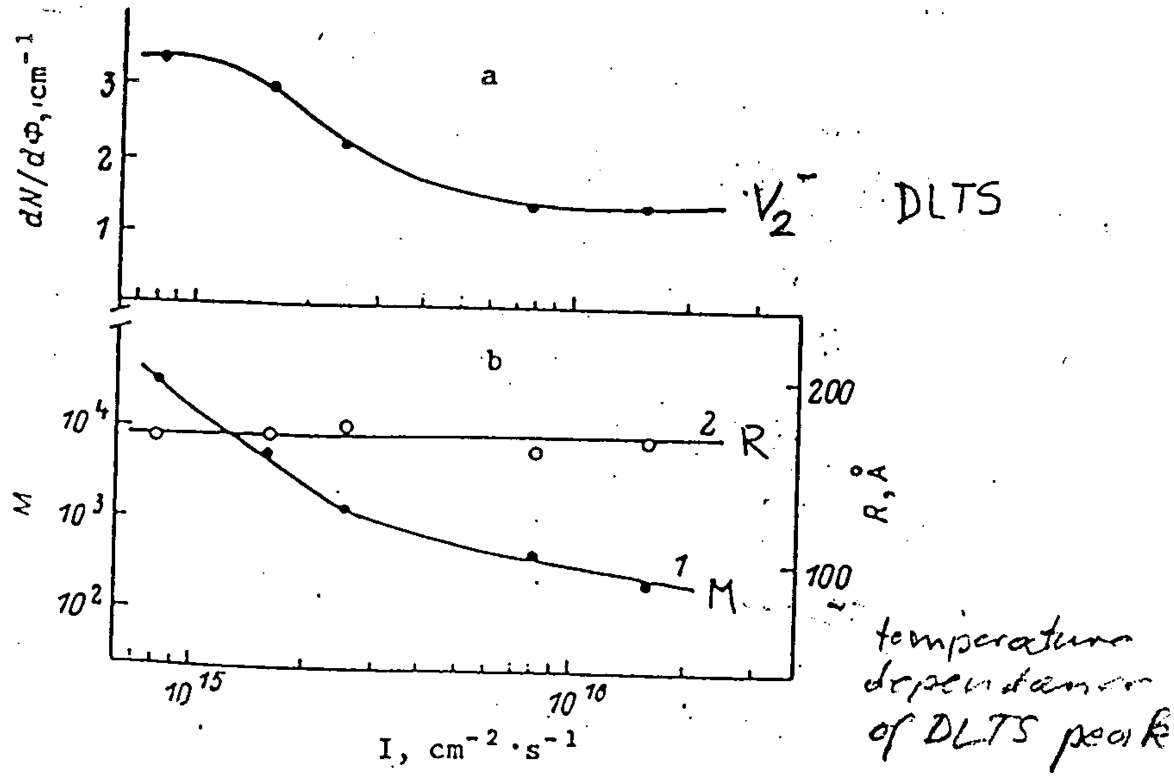
**4.1 Positive annealing: destruction of D in vacancies by C**

**4.2 Negative annealing : destruction of D in clusters by C**

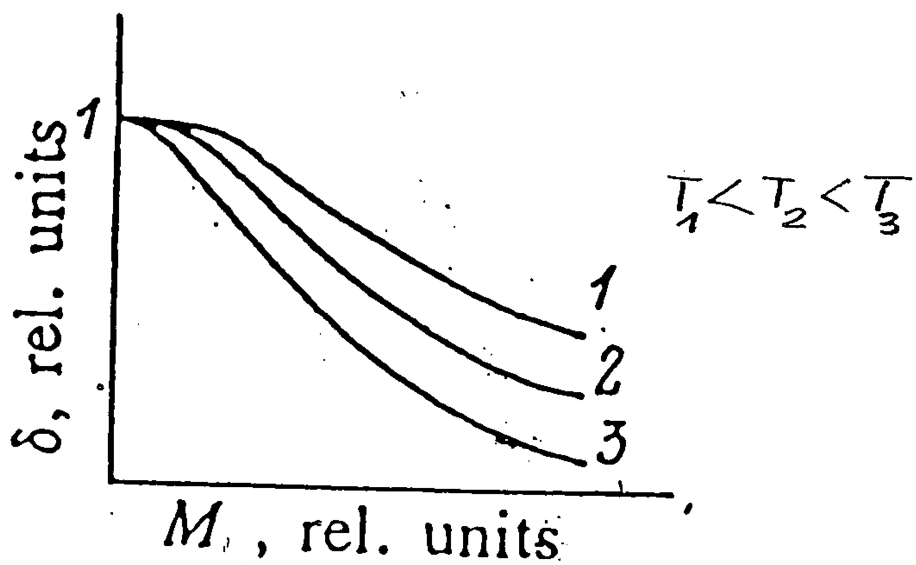
**Why??**

**Because destruction of D lowers potential barrier and more Charged D become visible**

I.V.Antonova et al. Sov.Phys.Semicond. vol.23 p 944 (1989)




I.V.Antonova and S.S. Shaimeev, Sov.Phys.Semicond. vol.25 p513 (1991)



I.V.Antonova et al. Sov.Phys.Semicond. vol.22 p630 (1988)

have shown that $\psi_{max} \sim \ln D$

if D goes down D goes up

since $\Delta \psi_{max} \sim \frac{\Delta D}{D}$

$\Delta\psi_{max}$ changes strongly when few D left

this is reason why negative annealing delayed

## 4.3 Some experimental facts in favor of model

4.31 decrease of overall D measured by positron lifetime and infrared technique during annealing

4.32 Thesis M. Moll (1999) p198

peak H(116K) ↑ assignment to $C_i^{+/0}$
because C pushed in by strain field and gets immobile

appearance of small peak $V_2^{=}$

$C_i O_i$ and probably $C_i C_s$ go up

Unexplained time behavior of reverse annealing

## 5,. Conclusion and Outlook

some properties of clusters are able to explain peculiar behavior of our measurements; it has to be proven that clusters produced in ROSE detectors behave as the ones found in low resistivity material in particular geometrical complications are expected due to the great Debeye length in ROSE detectors. (merging of the periphery of clusters)

qualitative picture: further thinking if correct; refine or amend

quantitative model : needs description of primary cluster with
input from experiment ( probably dedicated)
since cluster shape depends also on chemical impurities whole kinetic of V and I- diffusion must be implemented
Calculate cluster size and number of D
Do point defect kinects in periphery of cluster