Deep levels in the irradiated Si (WODEAN) samples

and the V6 cluster modeling

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A short declaration

- WODEAN program has proposed to investigate the similar samples by different methods and to create the “real” model of irradiated to different fluence Si.
- Each method it was included into the WODEAN program reflects the in a certain sense a different spatial volume of the sample:
  - Light absorption, luminescence, photoconductivity generation reflects the processes in any place of the sample
  - Conductivity measurements performed by the contact methods illustrate the properties of the conductivity channel, and by microwave absorption represent the integral properties of the mobile carriers measurement

The problems:

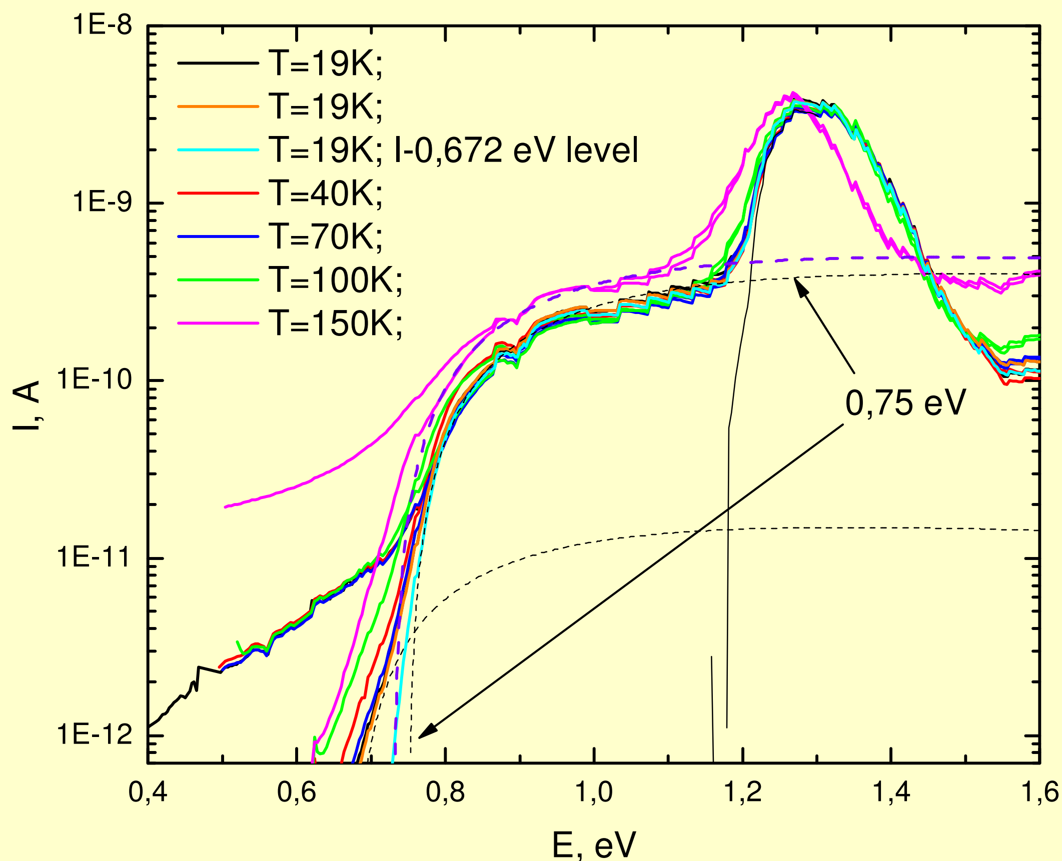
- The observed near to linear dependence of the free carrier lifetime on the fluence over the wide range of fluencies requests to discover the main recombination channel that is responsible for the lifetime.
- The observed data related to the avalanche process pay attention on the existence of the specific properties of the conductivity channels, therefore it is important to analyze obtained data more complex.

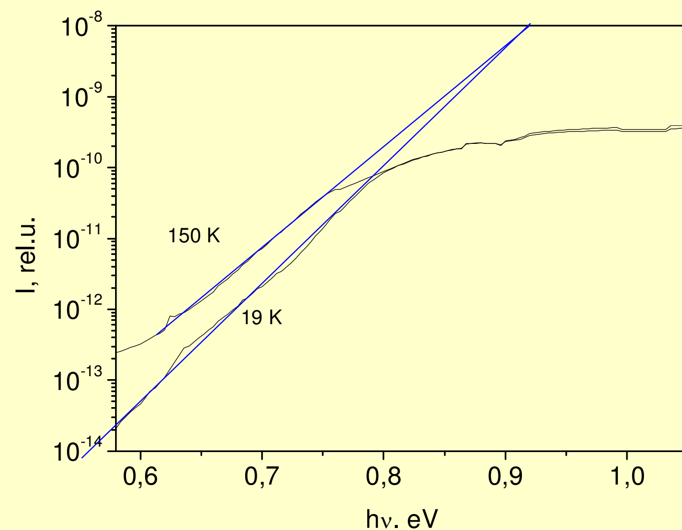
It follows that the complex analyze of the WODEAN samples data is still actual.

Outline of this talk:

- The presentation of:
  - the upgraded data of photoconductivity spectra in different samples.
  - The low temperature persistent current relaxation and its thermal stimulation
- The analyze of the structure of vacancy cluster in Si.
- The I-V modelling

PC at different T



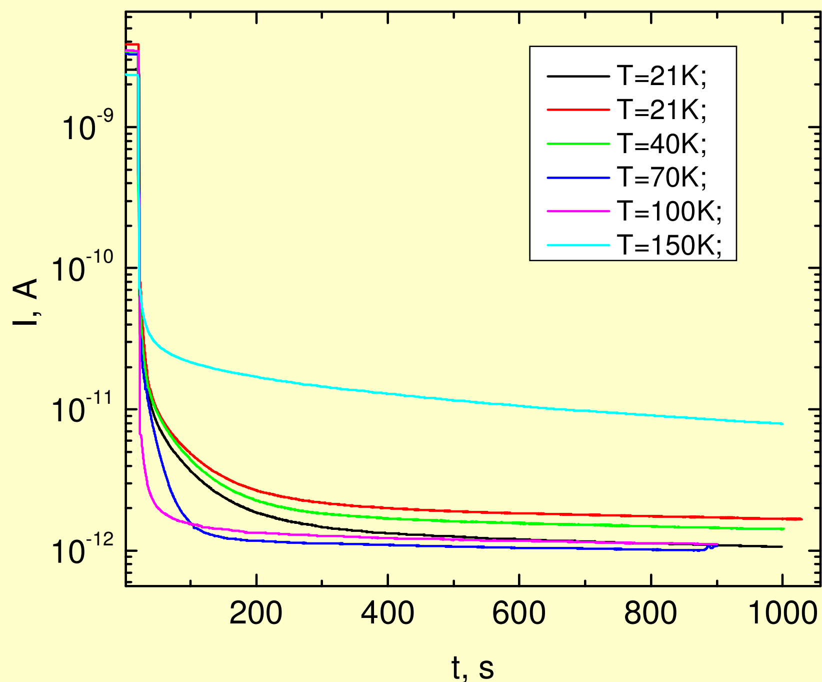


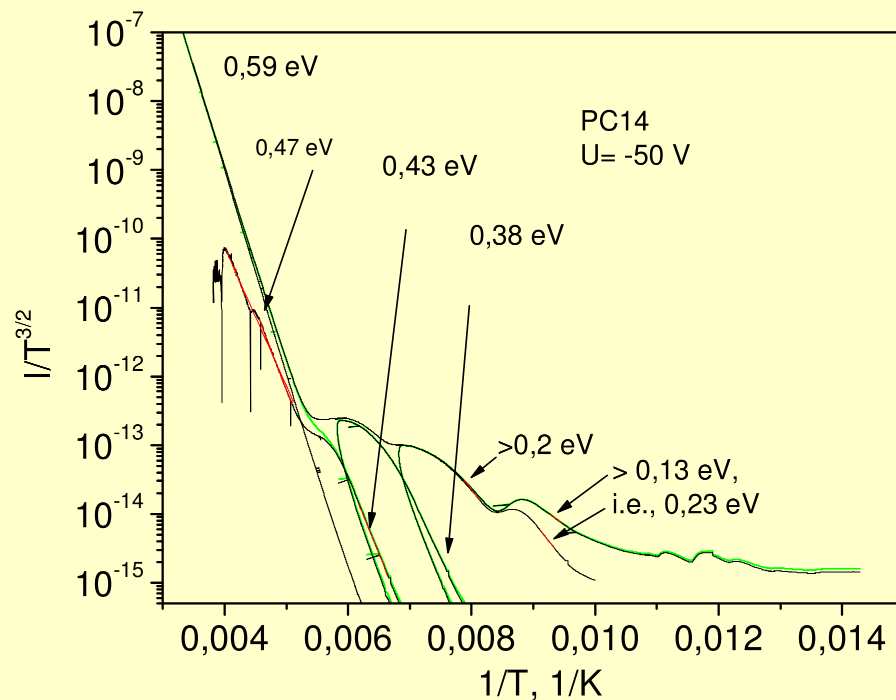
Electron-phonon coupling effect

The persistent current appears if the photon energy is bigger than 0.75 eV

Sample PC14 (8556-01-60), Triga reactor, neutrons 1e16 cm^{-2}

PC decay and TSC

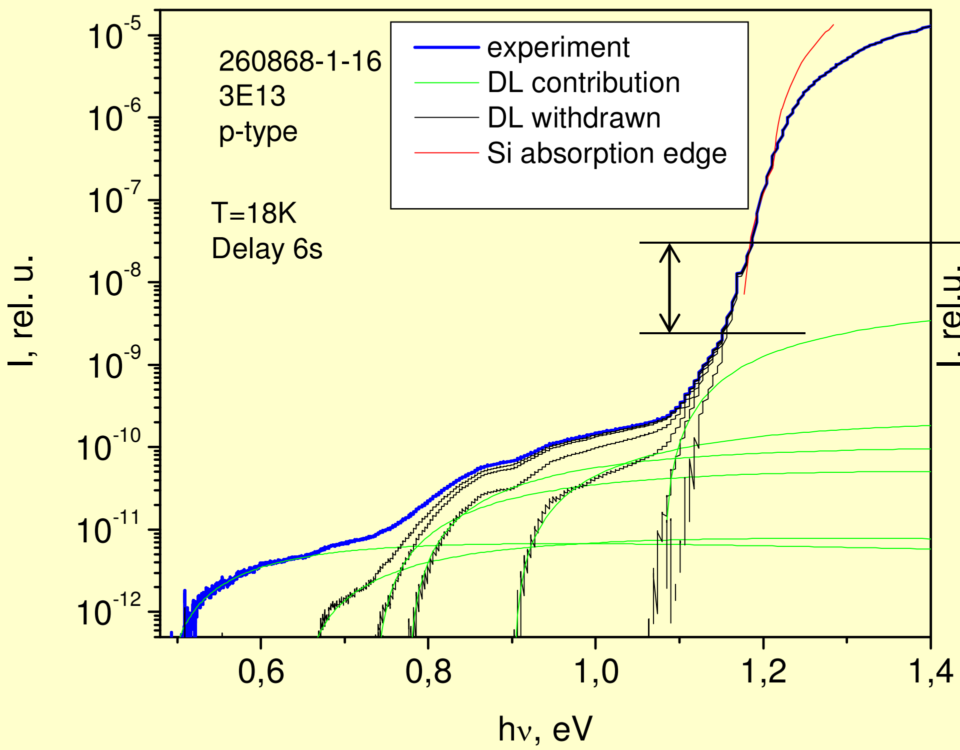


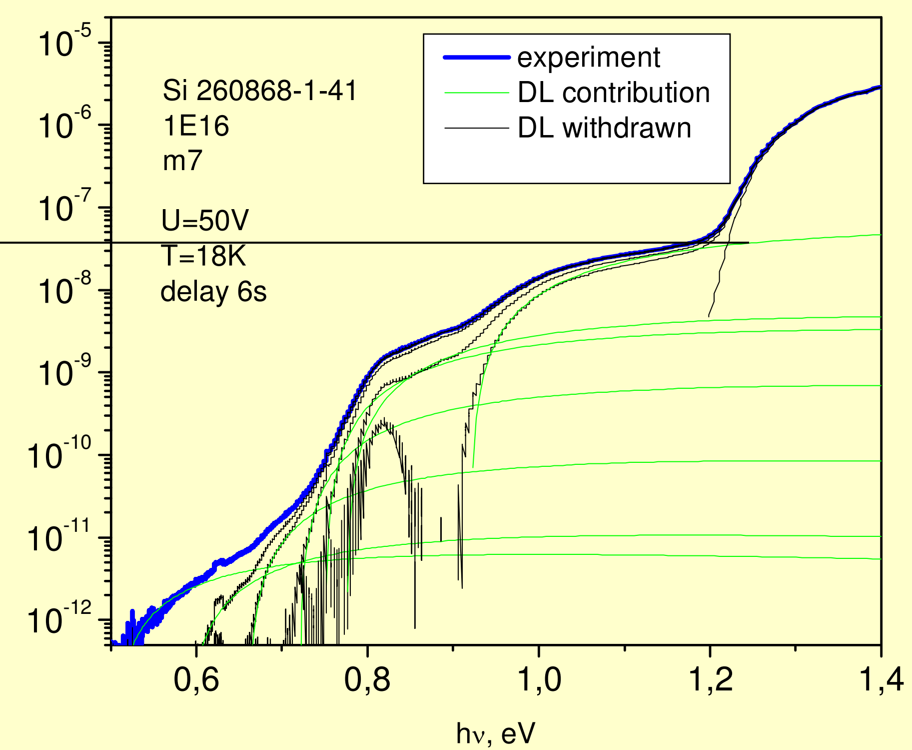


PC decay TSC

The excitation by 1,2 eV light

PC spectrum in p-type structure





PC spectrum in n-Si structure

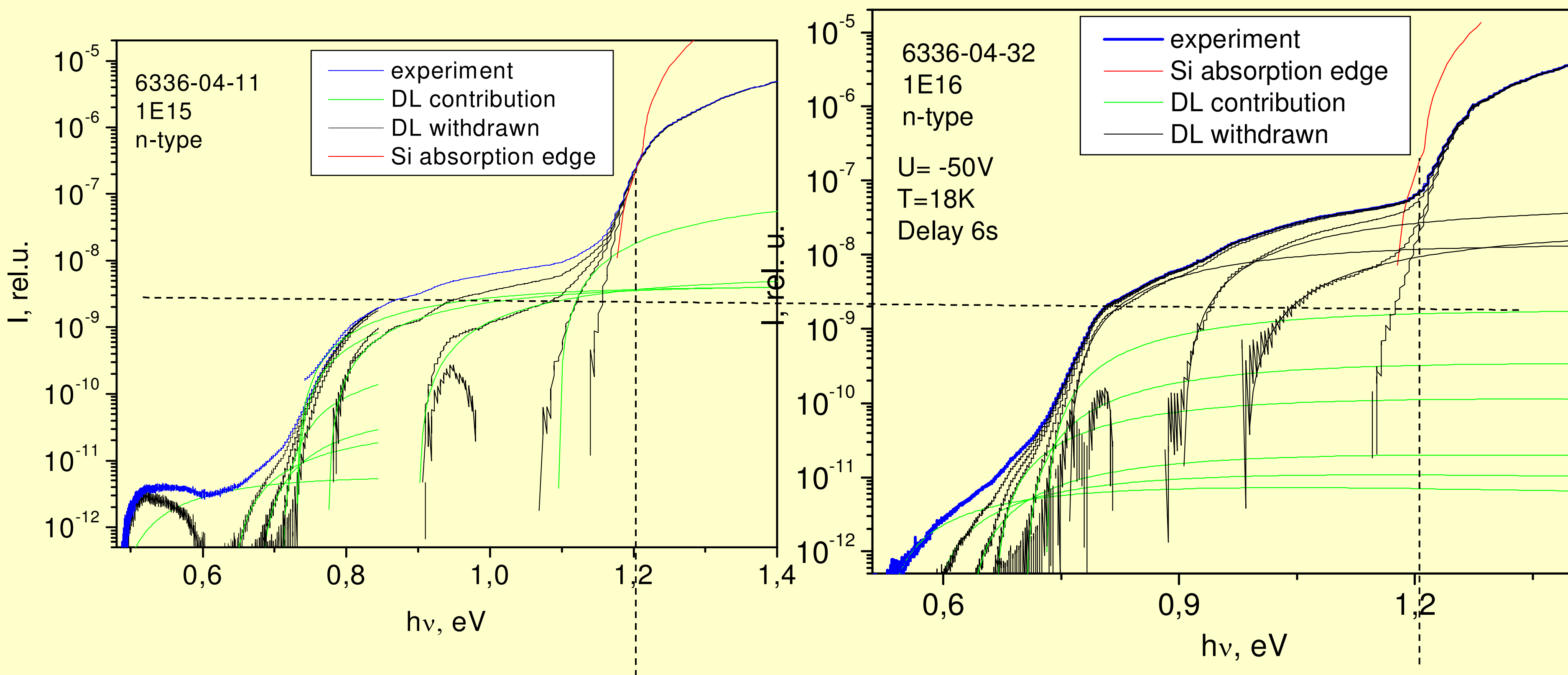


Photo-excitation of PC in the irradiated p- and n- Si

E_C
1,17 eV
E_V
P-type
N-type
14-181meV

Preliminary conclusion:

the PC spectra allow to recognize the deep level but there are absent the local level that influence directly depend on the fluence. The observed defects have another dependence on the fluence.

Clusters as the recombination centers

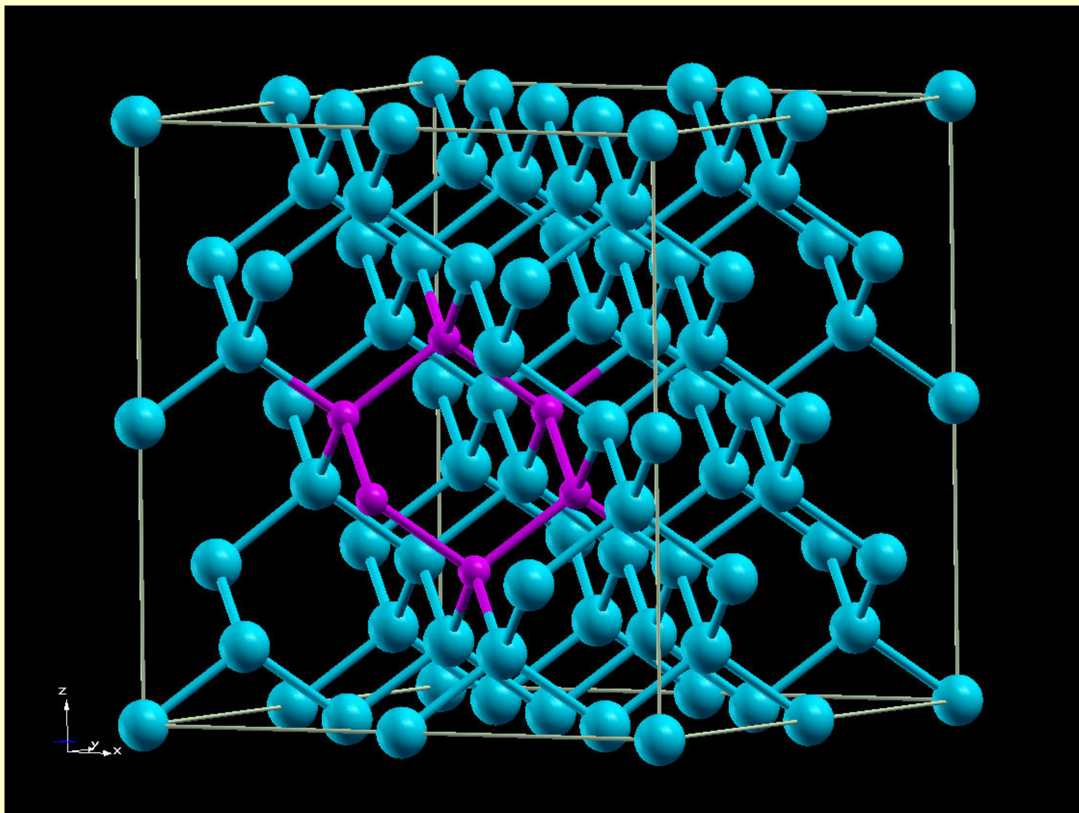
- As the recombination lifetime is inverse proportional to the fluence, the recombination rate can be defined as dependent on the distance between the effective recombination centers generated by the irradiation by hadrons.
- The hadron irradiation, due to the kick of Si ion, creates the clusters.
- Why do the clusters act as the effective recombination centers?

Model principle:

- It is known that at the surface due to the lattice relaxation the bandgap of Si is less than in the bulk.
- The vacancy is similar to the surface (Watson, Pantelides)
- The cluster created by the kicked-of Si-ion is formed by many vacancies.
- What properties have the clusters of vacancies including these that are electric inactive (V6)?

V6 deffect electronic and lattice structure

The 6 vacancies ring (V6) was modelled by embedding such a deffect into periodic 64 Silicon atoms supercell. To calculate a total energy of the atomic system, its relaxation and energy bands we applied density functional theory and used “Abinit” computer code [1]. The electronic wave functions were expanded in a plane-wave basis set with the kinetic energy cut-off 10 Hartree.



Ideal bulk positions of Si ions (cyan) and 6 vacancies (represented by magenta spheres) forming a ring.
(Magenta spheres and their links to Si ions are only for demonstration purpose.)

[1] Gonze X., *et al,* Computational Materials Science **25**, 478-492 (2002).

Basics of Density-Functional Theory [2]

Electron ground state wave function is found from the system of equations (the first one is called Kohn-Sham equation):

$$\left[\hat{T} + \hat{V}_H + \hat{V}_{ext} + \hat{V}_{xc}\right]\Phi_i = \varepsilon_i \Phi_i$$

$$n(\mathbf{r}) = \sum_i |\Phi_i(\mathbf{r})|^2$$

Total potential for electrons depends on their density *n*:

$$V(n,r) = V_H(n) + V_{ion}(r) + V_{xc}(n)$$

$V_H(n)$ – Hartree potential

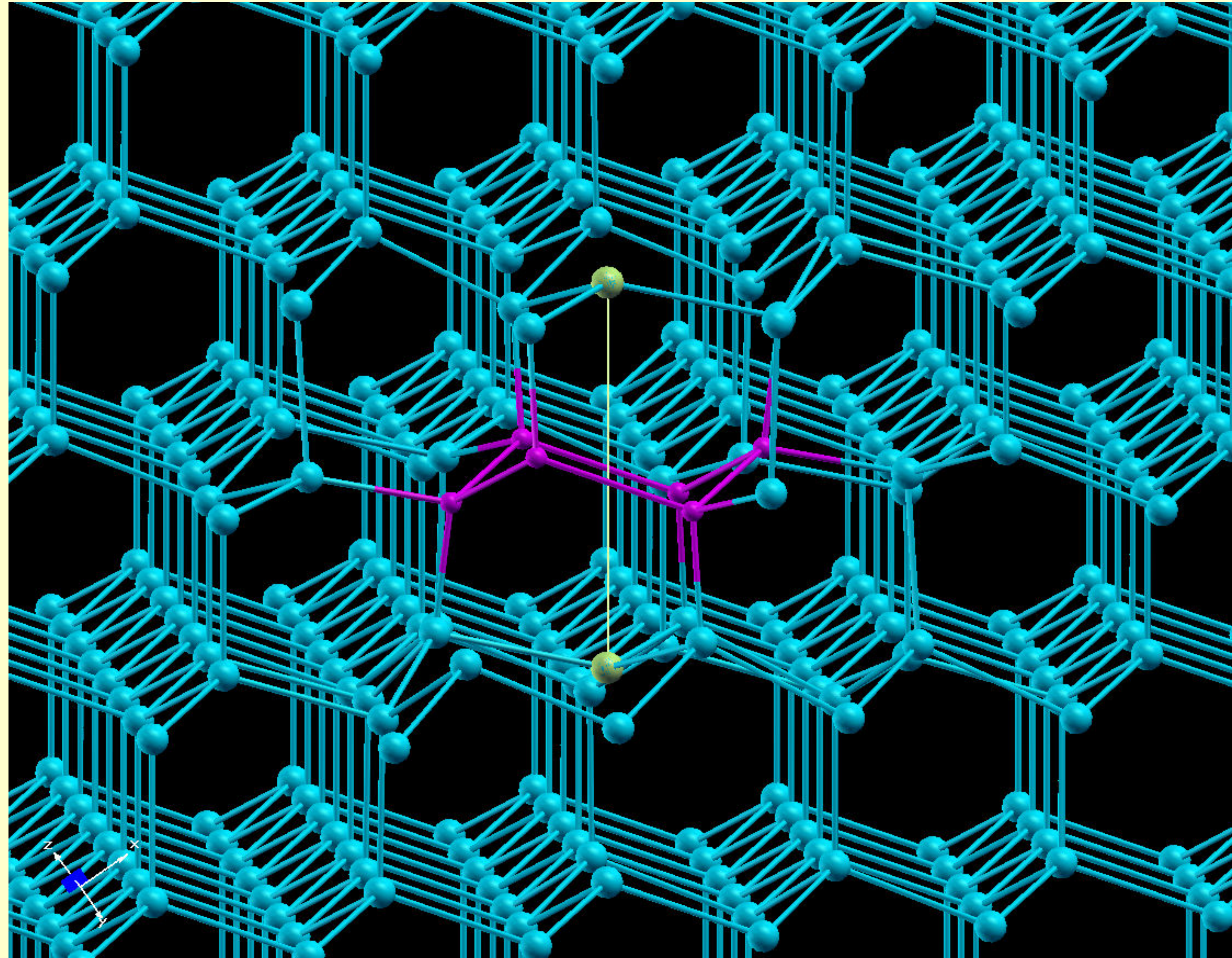
$V_{ion}(r)$ - ions potential (V_{ext})

$V_{xc}(n)$ – exchange-correlation potential

[2] W. Kohn, L. J. Sham, Phys. Rev. **140**, 1133, (1965)

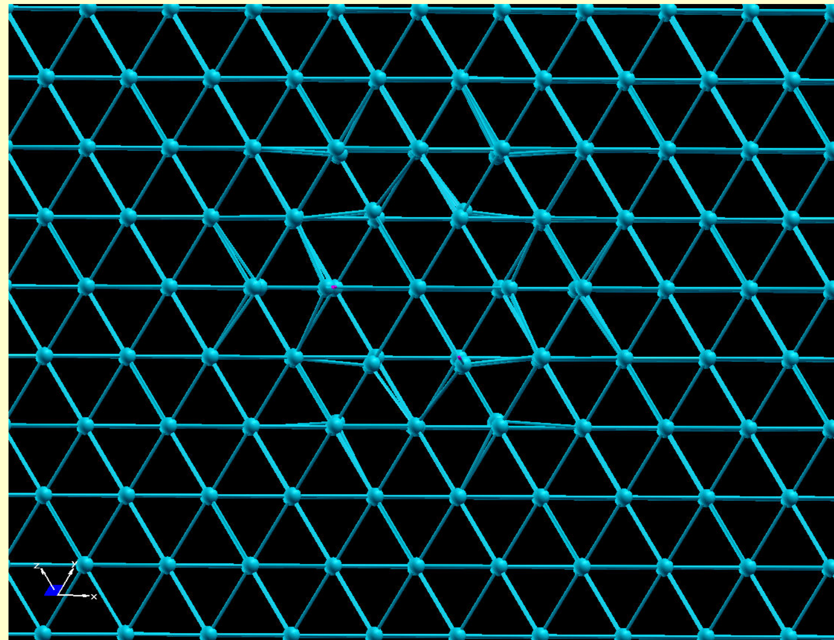
Lattice relaxation nearby V6

Two Si ions shown (yellow spheres) lie exactly on the symmetry axis of V6 ring (yellow line)

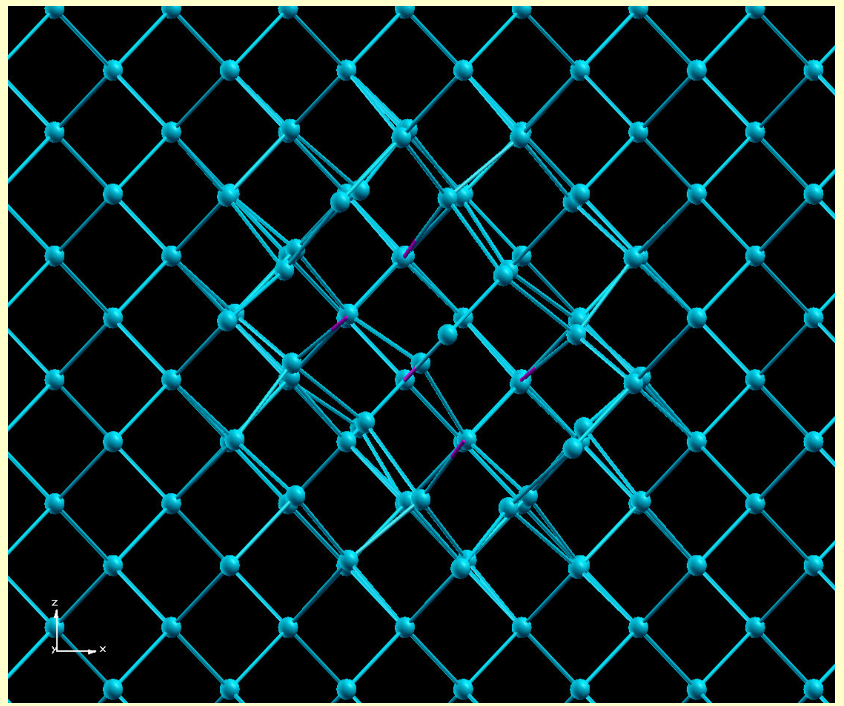


Only the nearest ant the next-nearest to vacancies ions were allowed to relax in simulation

Disturbance of periodic lattice structure by V6 seen

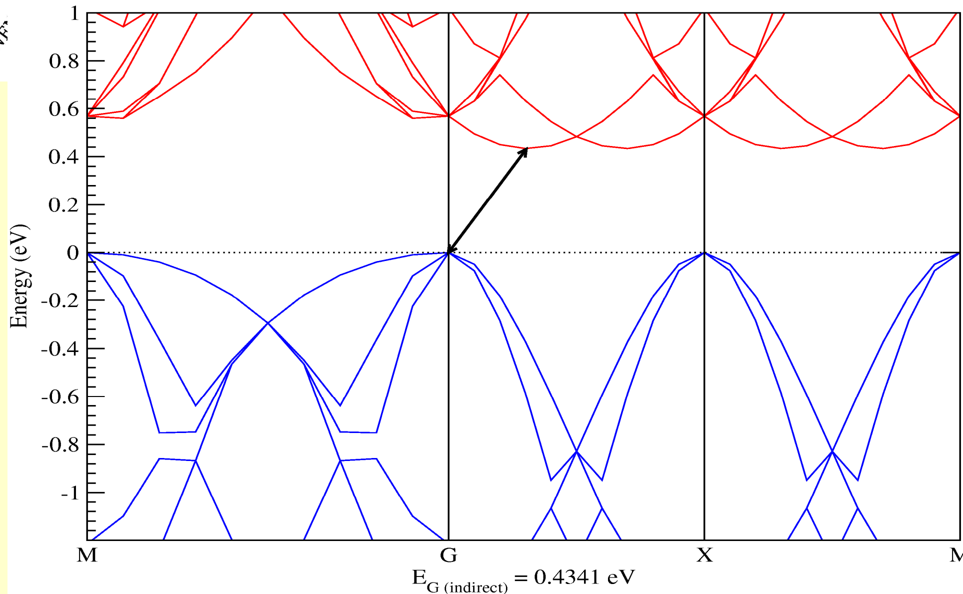


... from (111) direction



... and from (100) direction

Band structures found from Kohn-Sham equation (known to give wrong picture)



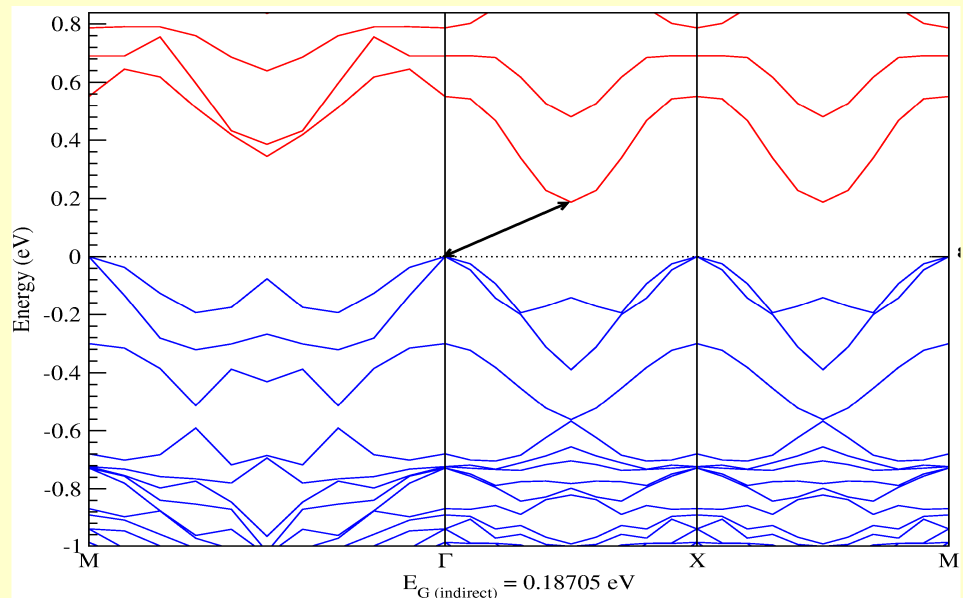
1. Wrong Gap values:

   $E_G = 0.434$ eV for bulk 64-Si

   $E_G = 0.187$ eV for bulk 64-Si-V6

2. Wrong Gap location: due to lattice doubling the X point folds into Gamma point, so the smallest gap must be located at the Gamma point

Corrections taking into account quasiparticle self-energy and potential screening must be done!



First but very rude (with only one k-point) calculations of the corrections to the band energies give:

$E_G = 3.1$ eV for bulk 64-Si

$E_G = 1.8$ eV for bulk 64-Si-V6

TENDENCY IS THE SAME !!!

GAP DECREASES

Next conclusion:

- If the vacancy cluster is surrounded by the more narrow bandgap as in the bulk, then this cluster acts as the attractor of both carriers, and therefore the clusters are the effective recombination centers.
- The photoconductivity spectra reveal the generation of carriers from the deep level both in the cluster and in the bulk part of the crystal.

Additional analyze

- The change of deep level concentration influence on the space charge distribution and the current, i.e., I-V
- The I-V simulation was performed for some cases

An example of I-V in irradiated n-Si structure

6336-04
n-type

T=300K
0,1V/s

abs I (A)

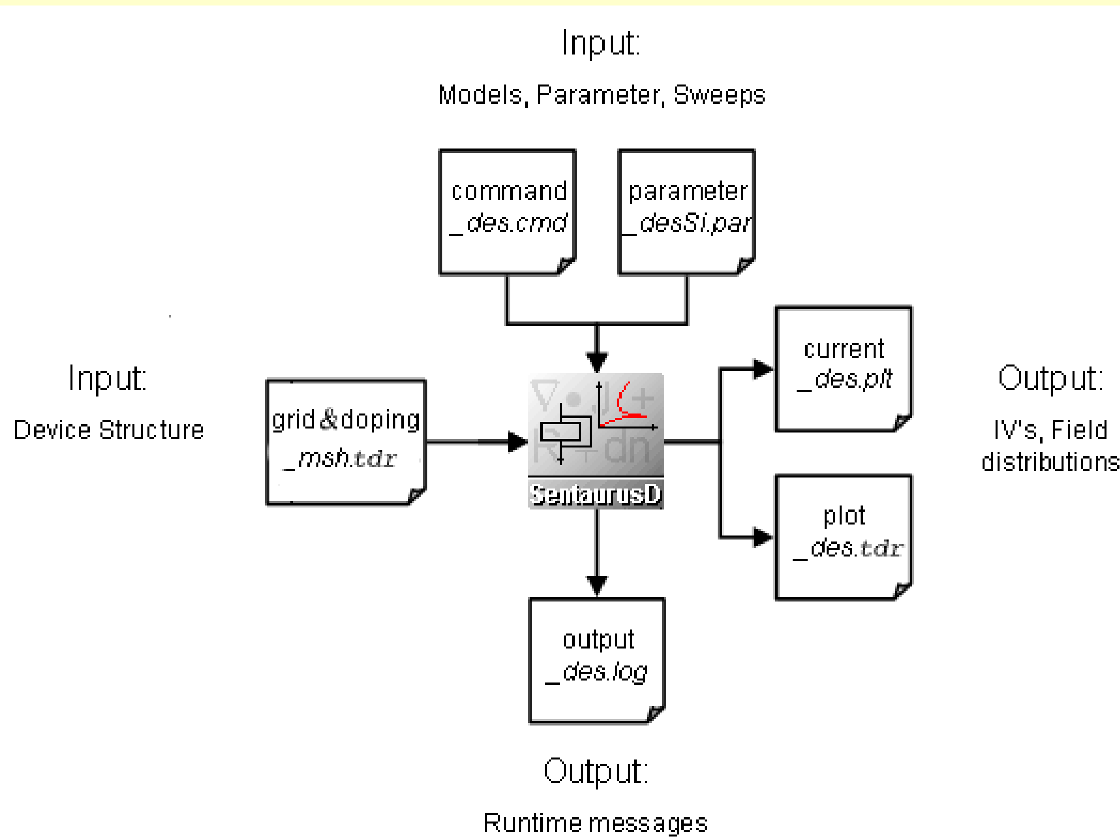
10^{-4}
10^{-5}
10^{-6}
10^{-7}

1e16 cm^{-2}
1e15 cm^{-2}
2e-14 cm^{-2}

-100 -80 -60 -40 -20 0,01 0,1 1

U (V)

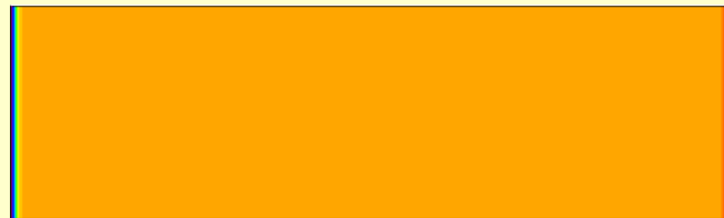
Device Modeling With Sentaurus Device



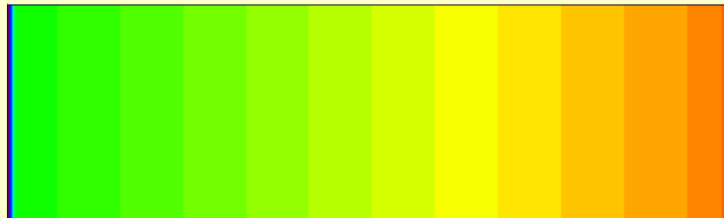
Synopsys TCAD tools:

- Sentaurus Process
- Sentaurus Structure Editor
- Sentaurus Device
- Plot and inspect tools

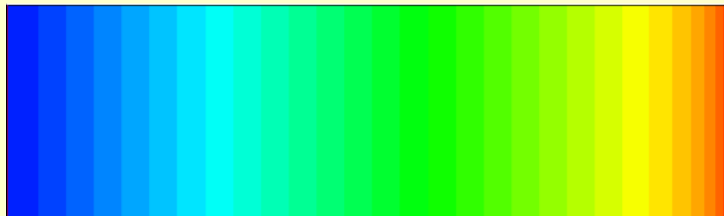
Potential distribution in *pnn⁺* diode



U = 0.0 V

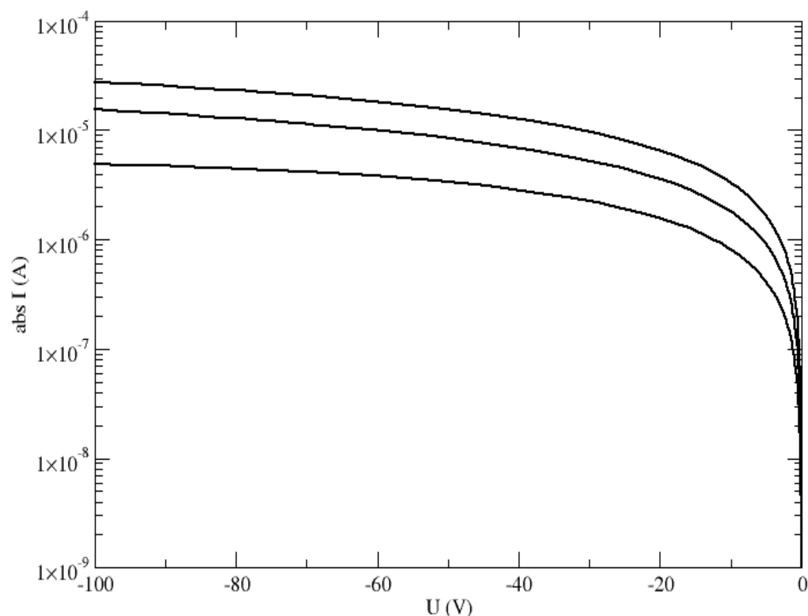


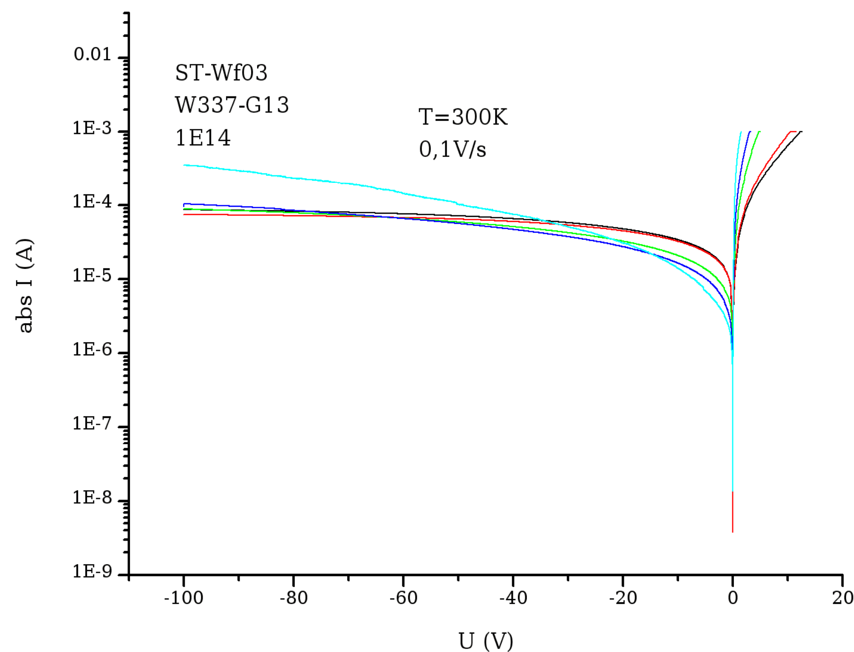
U = 100 V



U = 600 V

I-U characteristics of modeled *pnn⁺* diode



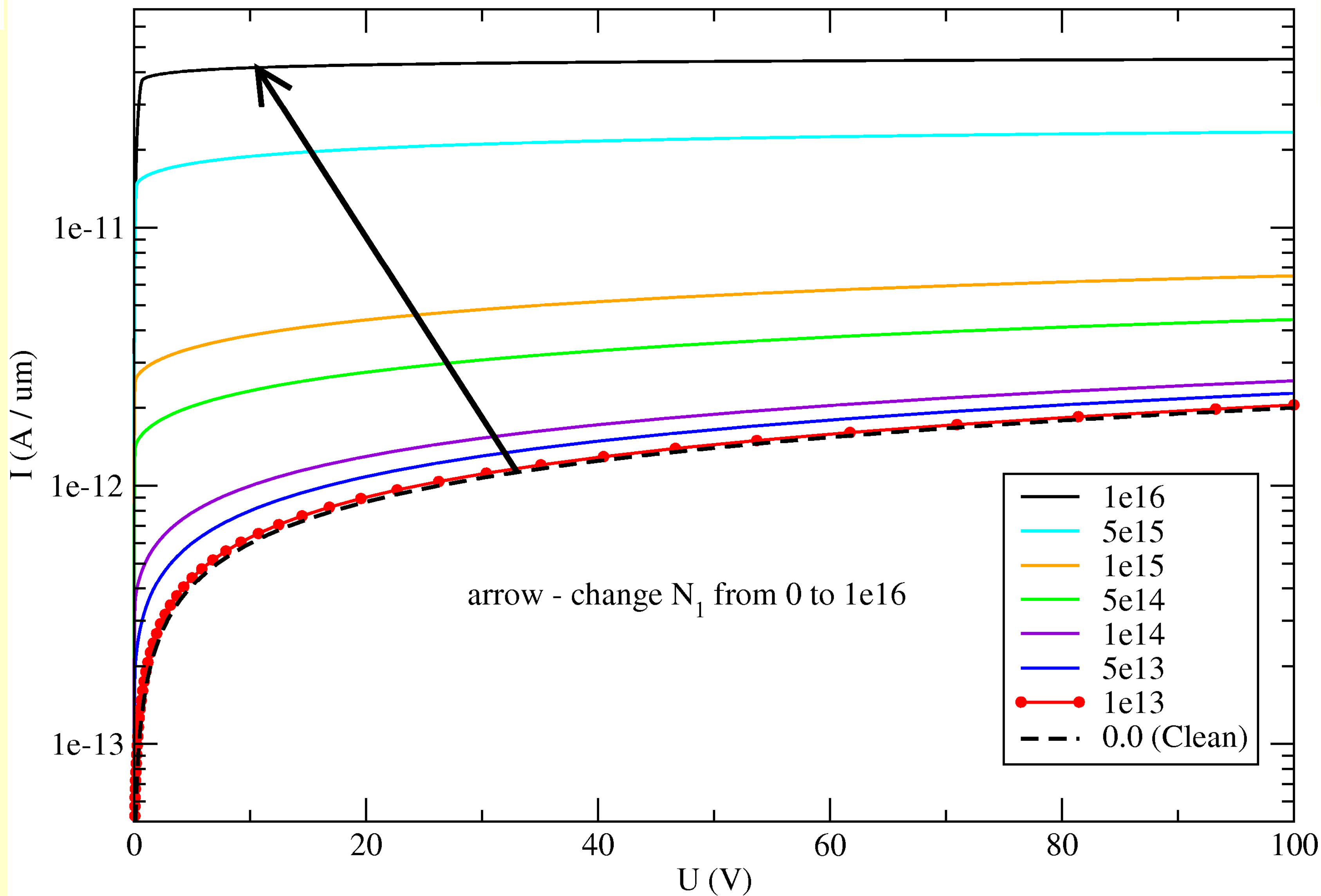


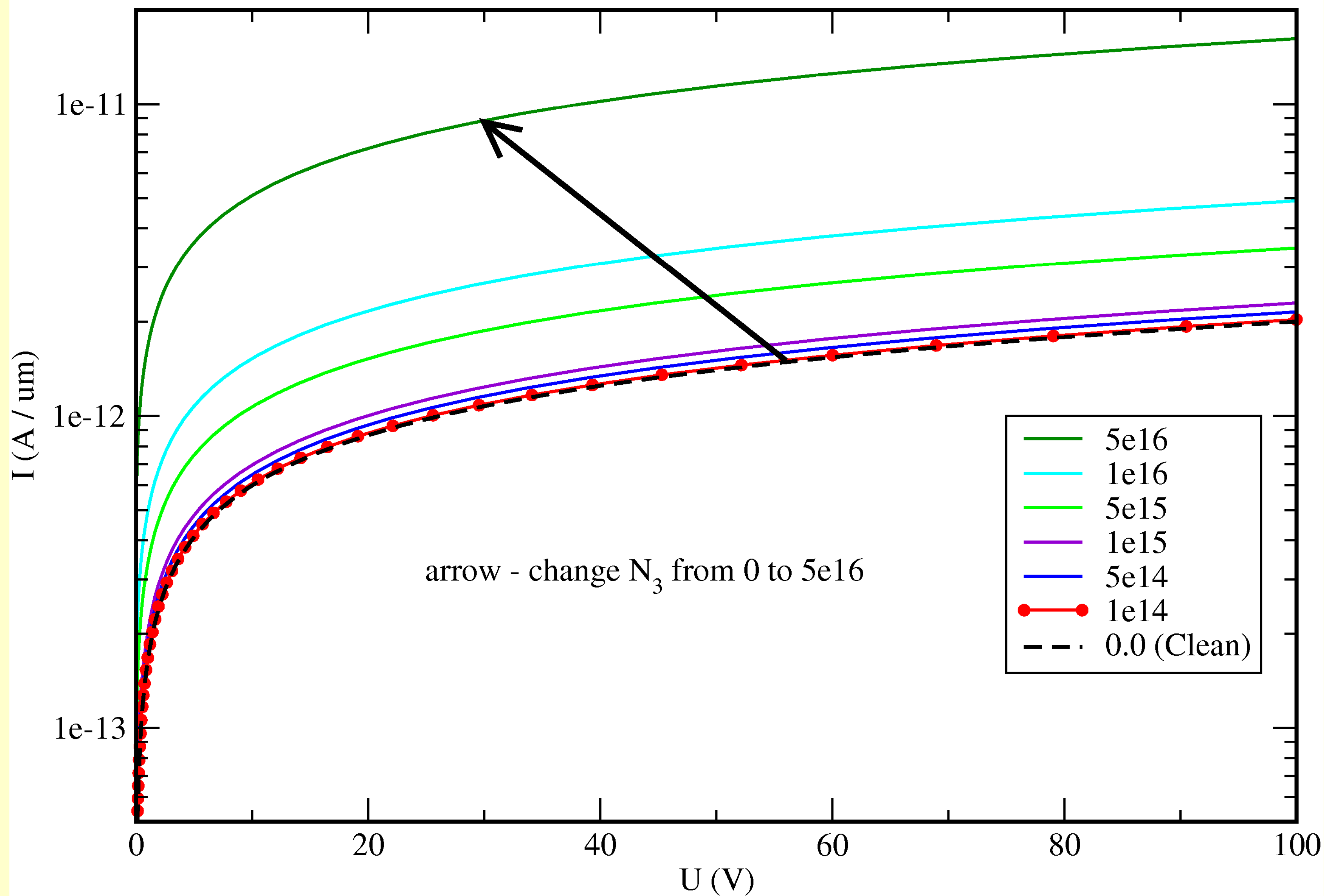
Modeled I-U curves. Attempt to modell the annealing effect by changing the width of the trap levels from 0 eV (bottom curve) to 0.2 eV (top curve). Model of the traps is given by D. Passeri, P. Ciampolini, G. Bilei, and F. Moscatelli, IEEE Trans. Nucl. Sci., **48**, 1688, (2001)

Measured I-U charecteristics of the sample after the various times of annealing

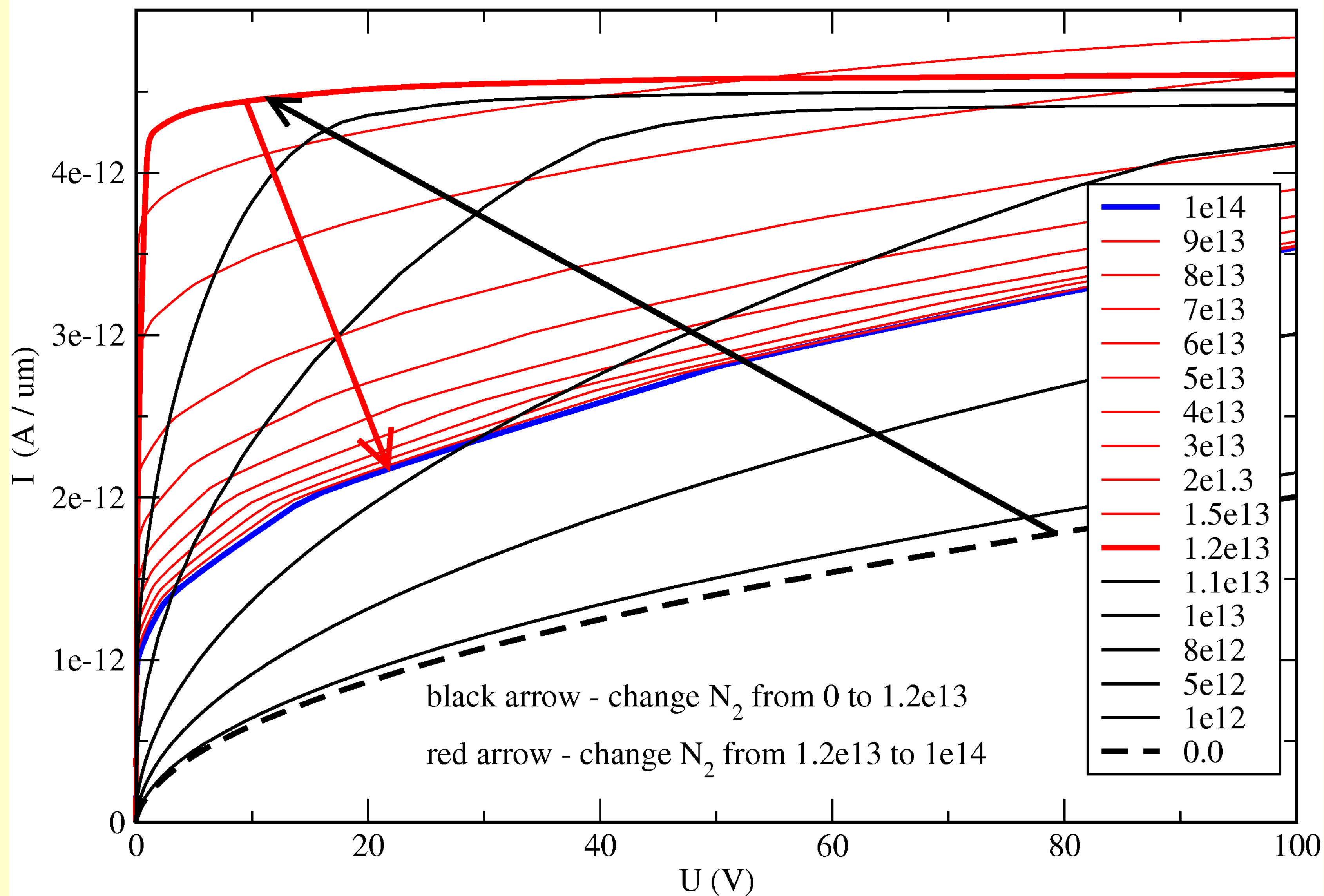
Modelled trap system

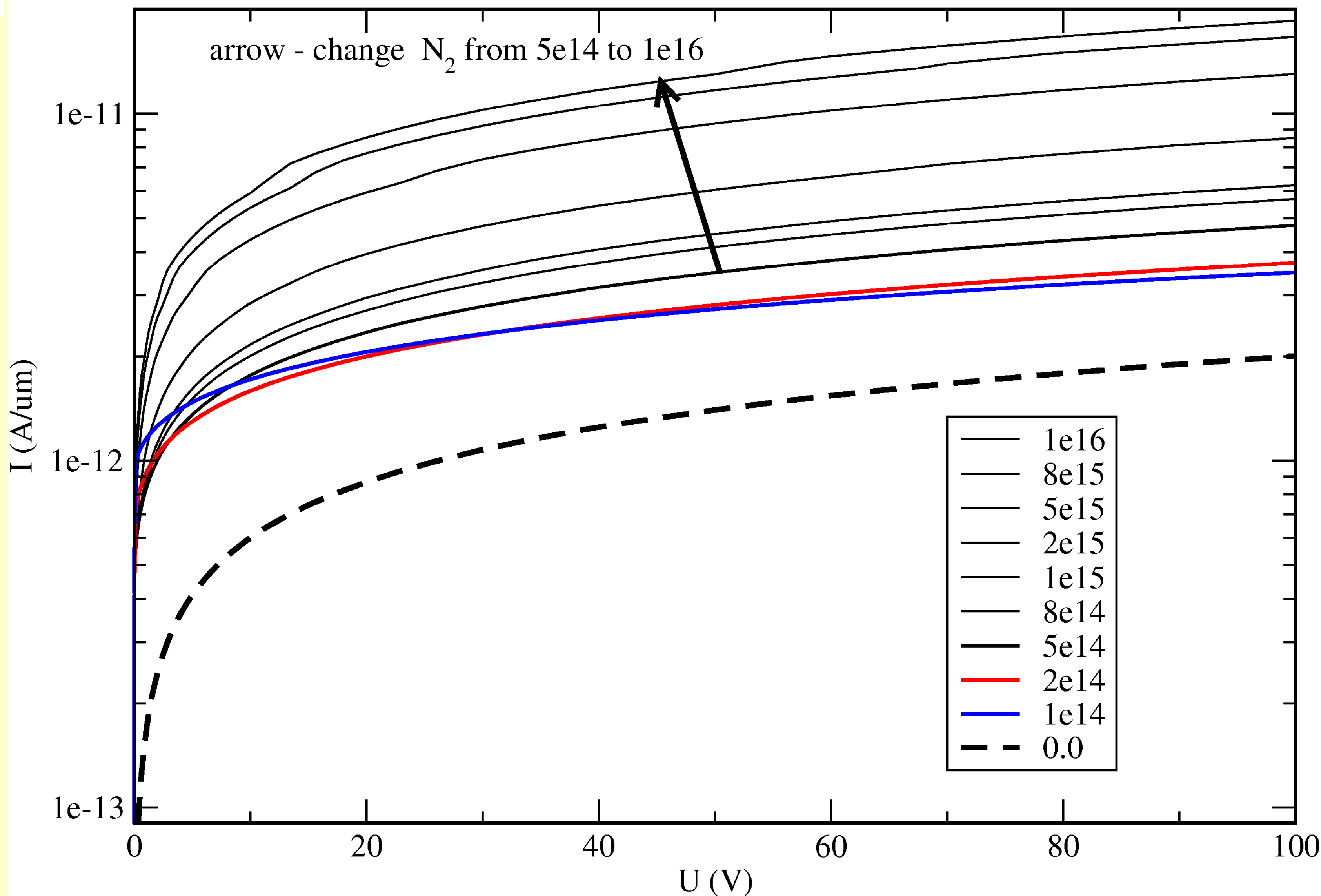
	Type	Energy (eV)	N-section (cm^2)	P-section (cm^2)
1	Acceptor	$E_c - 0.42$	10^{-14}	10^{-15}
2	Acceptor	$E_c - 0.55$	10^{-16}	10^{-15}
3	Donor	$E_v + 0.36$	10^{-15}	10^{-16}


I-V plots at $N_2 = 0$, $N_3 = 0$, variable N_1
1e-11
1e-12
1e-13
I (A / um)
0
20
40
60
80
100
U (V)
arrow - change N_1 from 0 to 1e16
1e16
5e15
1e15
5e14
1e14
5e13
1e13
0.0 (Clean)



I-V plots at $N_1 = 0$, $N_2 = 0$, variable N_3
1e-11
1e-12
1e-13
I (A / um)
0
20
40
60
80
100
U (V)
5e16
1e16
5e15
1e15
5e14
1e14
0.0 (Clean)
arrow - change N_3 from 0 to 5e16


I-V plots at N1 = 0, N3 = 0, variable N2
I (A / um)
U (V)
4e-12
3e-12
2e-12
1e-12
0
0
20
40
60
80
100
1e14
9e13
8e13
7e13
6e13
5e13
4e13
3e13
2e1.3
1.5e13
1.2e13
1.1e13
1e13
8e12
5e12
1e12
0.0
black arrow - change N2 from 0 to 1.2e13
red arrow - change N2 from 1.2e13 to 1e14


I-V plots at $N_1 = 0$, $N_3 = 0$, variable N_2
arrow - change N_2 from 5e14 to 1e16
1e-11
1e-12
1e-13
I (A/um)
0
20
40
60
80
100
U (V)
1e16
8e15
5e15
2e15
1e15
8e14
5e14
2e14
1e14
0.0

I-V plots at N_1 = 1e15, N_3 = 1e15, variable N_2

black arrow - change N_2 from 0 to 1.2e13 (thick curves)

blue arrow - change N_2 from 1.2e13 to 3e14 (dashed curves)

red arrow - change N_2 from 3e14 to 1e16 (thin curves)

Legend: 1e16, 5e15, 2e15, 1e15, 5e14, 3e14, 1e14, 5e13, 3e13, 2e13, 1.5e13, 1.2e13, 1e13, 9e12, 5e12, 1e12, 0.0, Clean

I (A / um): 0, 1e-11, 2e-11

U (V): 0, 20, 40, 60, 80, 100

Part of the Slide 6

I-V plots at N_1 = 1e15, N_3 = 1e15, variable N_2

black arrow - change N_2 from 0 to 1.2e13 (thick curves)

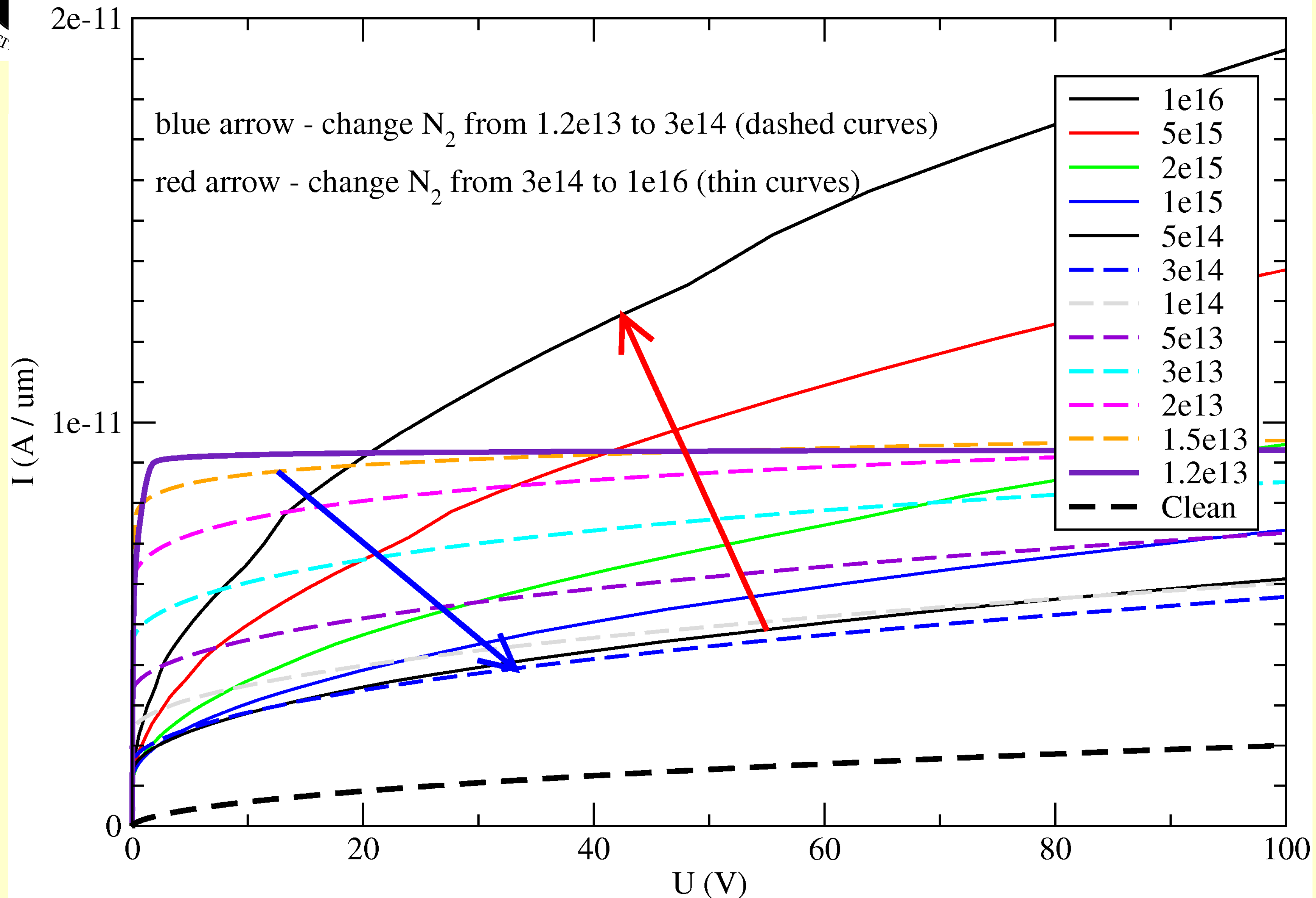
blue arrow - change N_2 from 1.2e13 to 3e14 (dashed curves)

Legend: 3e14, 1e14, 5e13, 3e13, 2e13, 1.5e13, 1.2e13, 1e13, 9e12, 5e12, 1e12, 0.0, Clean

I (A / um): 0, 1e-11, 2e-11

U (V): 0, 20, 40, 60, 80, 100

Another part of the slide 6



Instead of conclusion:

- Most of modelling was performed for homogeneous structure cases, it is necessary to analyze more complicated channels of conductivity in semiconductor.
- The clusters – attractors can cause the fast recombination and the fast trapping. The concequences:
  - It is necessary to measure carefully the absorption edge in the irradiated Si (It was planned in WODEAN program);
  - It is necessary to investigate the ways to decrease the capture of one of carriers in the cluster to improve the properties of irradiated Si.

Thank You for attention !

Sentaurus Process is a multidimensional, process modeling program. Calibrated to a wide range of the latest experimental data ***Sentaurus Process*** offers predictive capabilities for the lots of technological processes like implantation, depositioning, etching, annealing and many others.

Sentaurus Structure Editor is a semiconductor device designing tool having a rich choice of built-in and materials used for device production, flexible tools for device parts drawing, and interactive interfaces for doping profiles creation. It has three distinct operational modes: 2D structure editing, 3D structure editing, and 3D process emulation. User-defined dopants and traps optionally distributed in the space may also be taken into account

Sentaurus Device is a modeling program used to compute the electrical, thermal and optical characteristics of silicon-based and compound semiconductor devices. It simulates 1D, 2D, and 3D geometries over a wide range of operating conditions, including mixed-mode circuit simulation, combining numeric devices with compact models. Program solves the standart set of device modeling equations with the possibility to include a vast theoretical models of semiconductor physics whenever needed.