# Modeling Vacancy-Interstitial Clusters and Their Effect on Carrier Transport in Silicon

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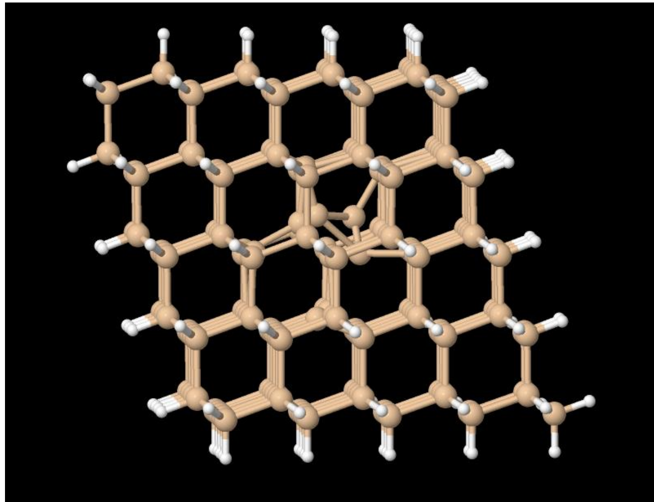
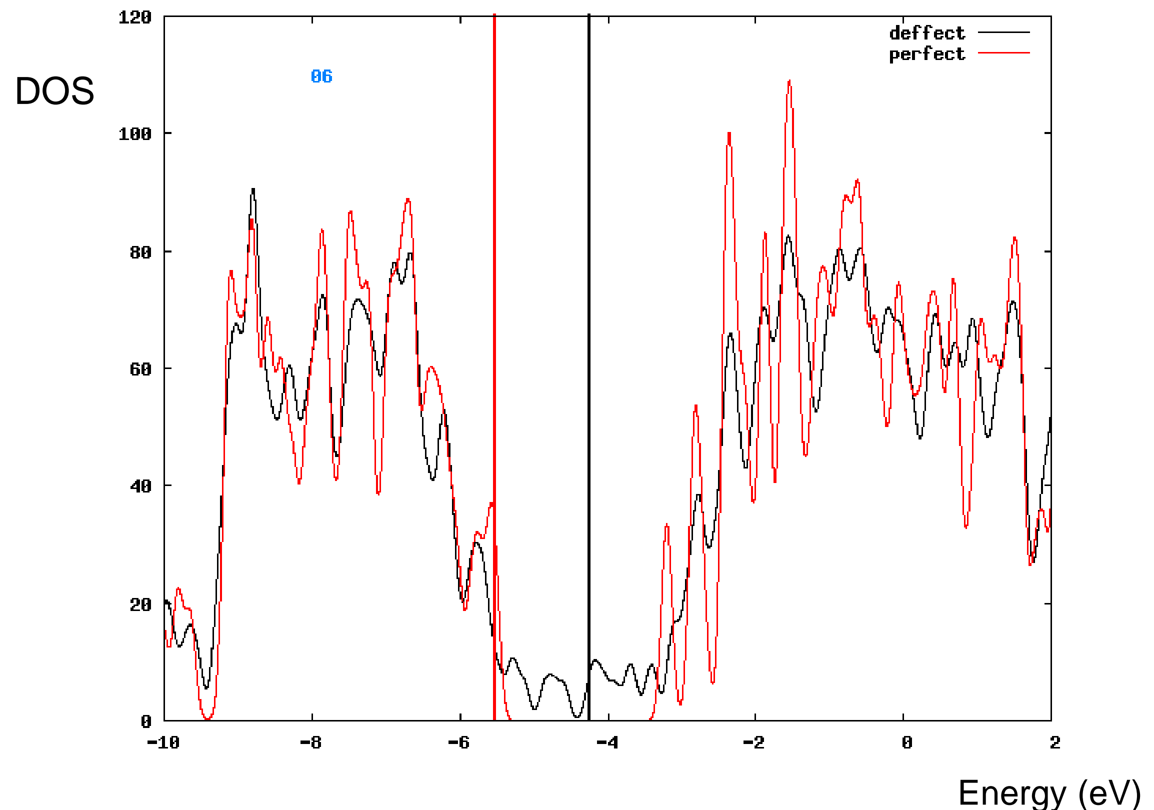
Cluster of intersititial and vacancy defects is modeled as a region of randomly displaced atoms from their crystaline positions.



Example of defect cluster:
Number of atoms displaced – 17
Size of cluster ~2 nm

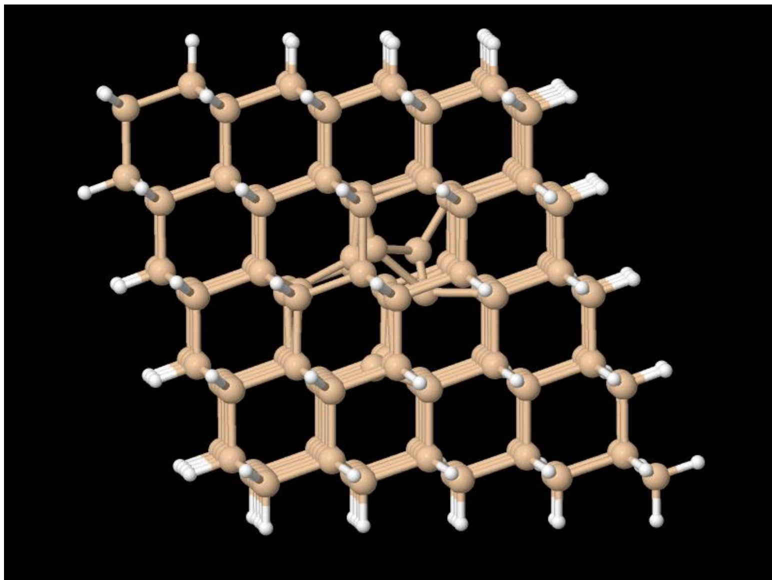



Density of electron states (DOS) in crystal with defect clusters (black) compared with the one in perfect crystal (red). Vertical lines indicate the highest energy level occupied states. DOS is calculated for 25 different randomly generated defect clusters.

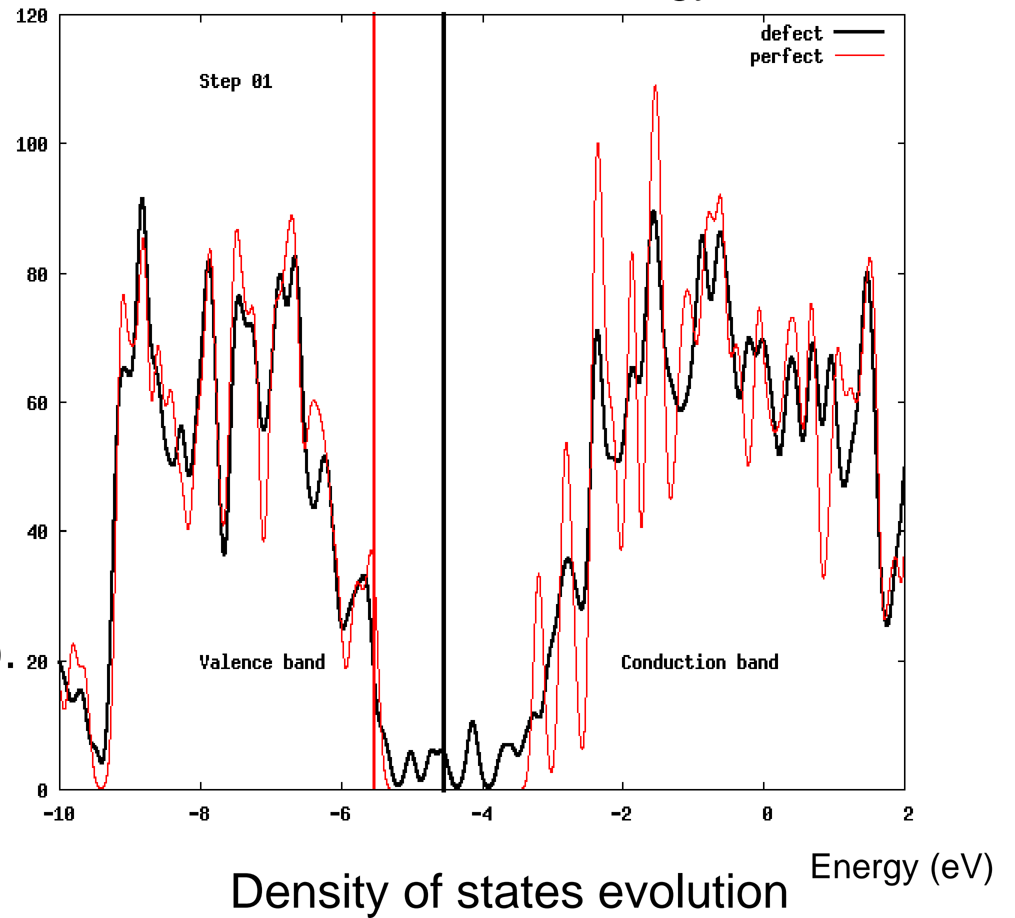
<u>All defect clusters have states with energy levels in band gap !</u>

*Density functional calculations were performed on* $\boldsymbol{C_{165}H_{100}}$ *cluster with ORCA program (F. Neese, MPI) using BP86 exchange correlation potential and and SVP basis function*

Selected example of defect cluster structure which relaxes to extended defect. Simultaneously are shown development of structure, its total energy and DOS

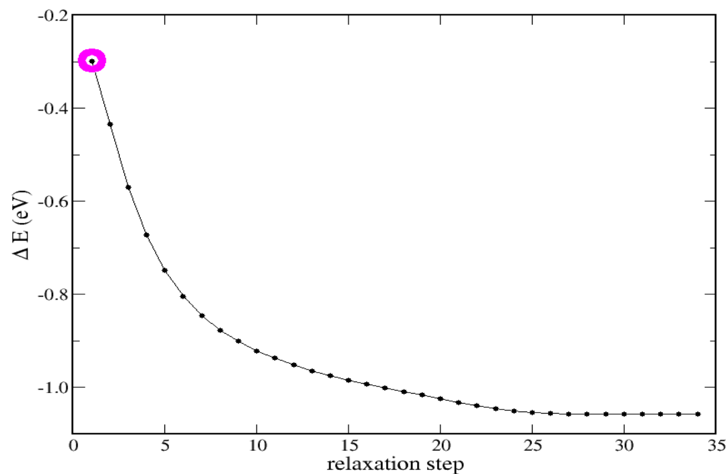


Structure relaxation (DFT simulation).

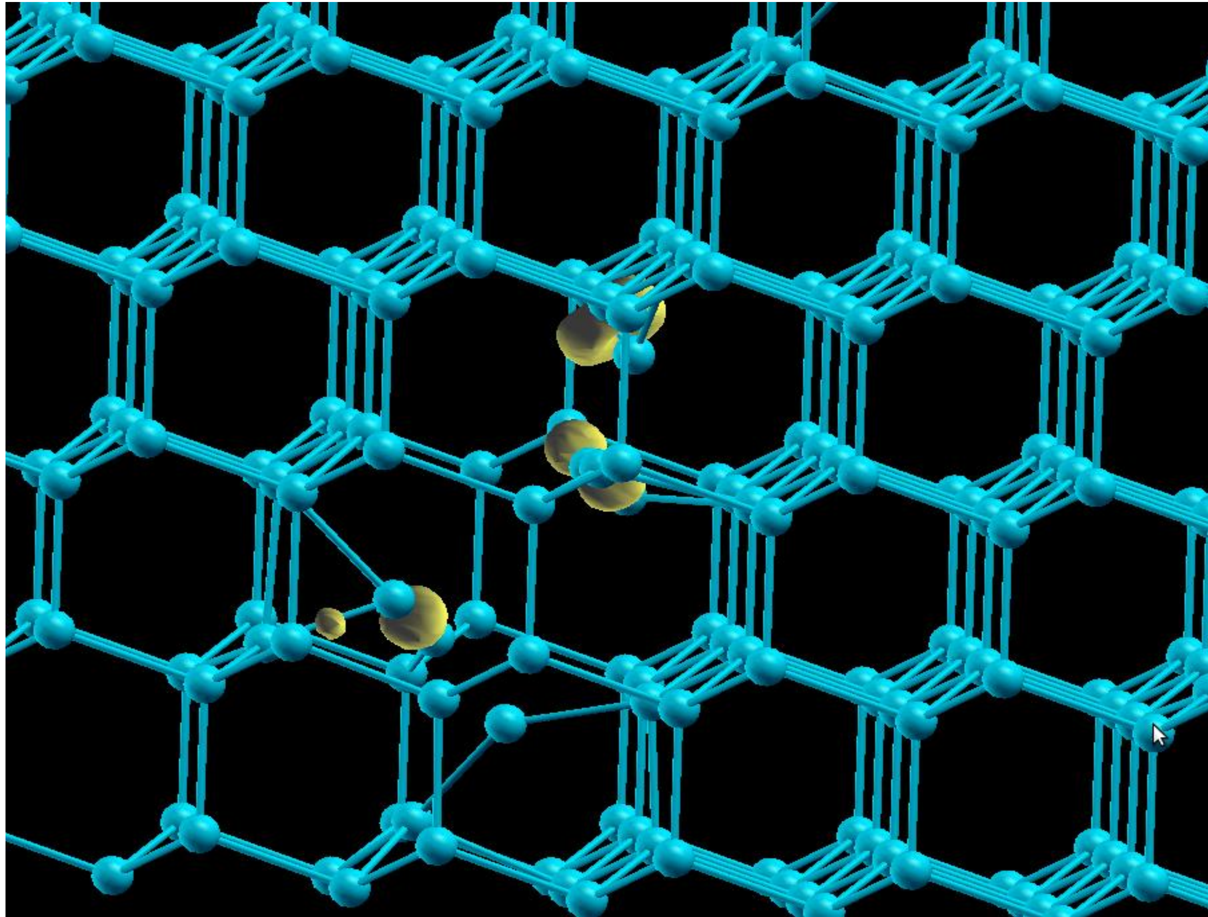



Energy (eV)

Density of states evolution

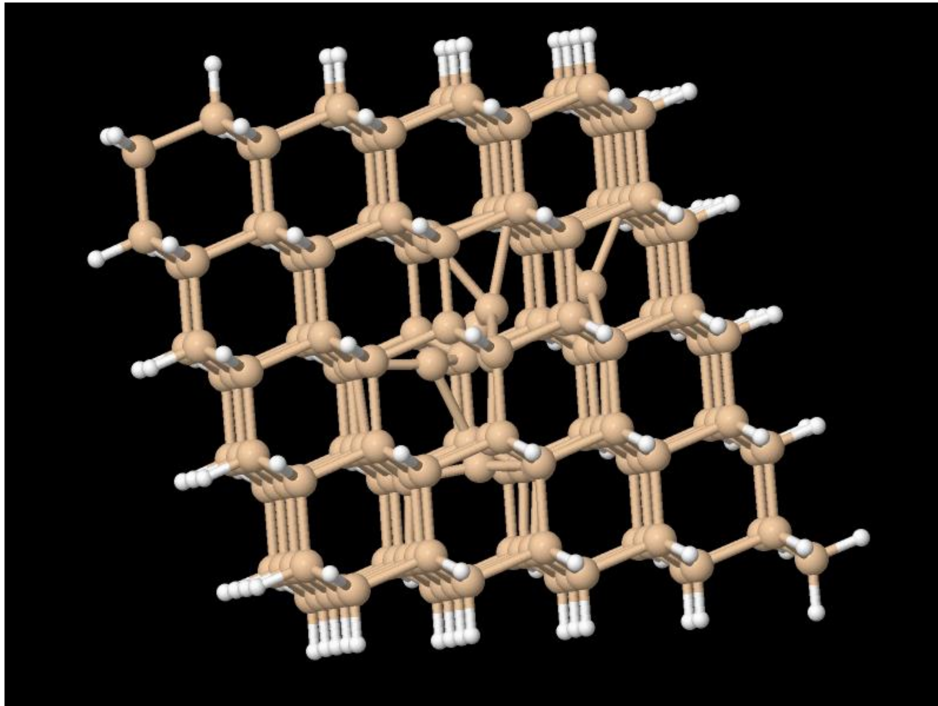


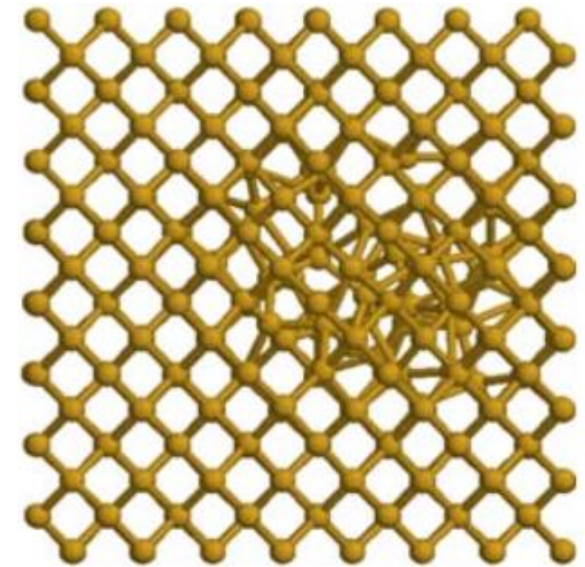

Total energy convergence



Trapped electron charge  distribution (yellow) within the acceptor type cluster defect.

Selected example of defect cluster structure which relaxes to perfect crystal (Annealing)





E. Holmström et al, Phys. Rev. B 82, 104111 (2010)

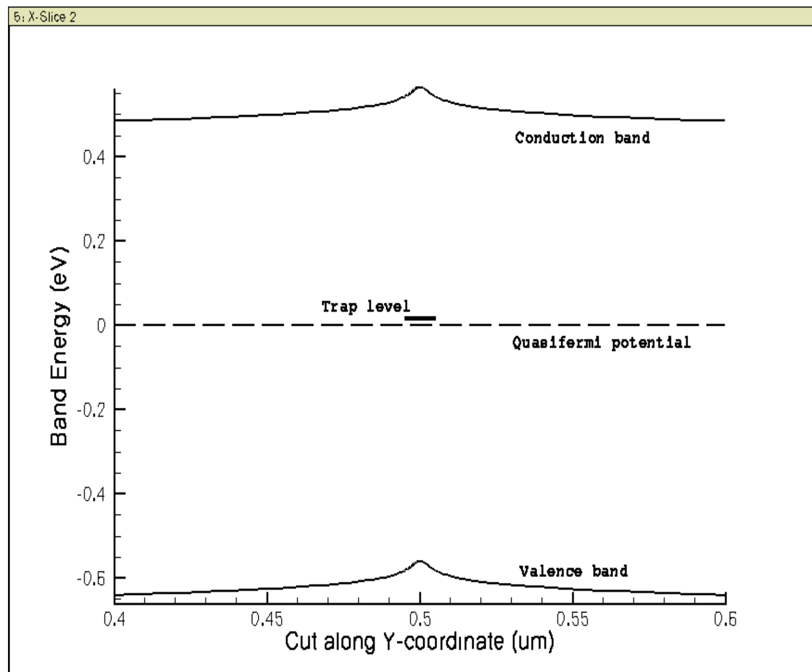
***This part of investigation was funded by EU structural assistance for Lithuania project " Radiation nanoclusters in Si and GaN" (VP1-3.1-ŠMM-07-K-03-010)***

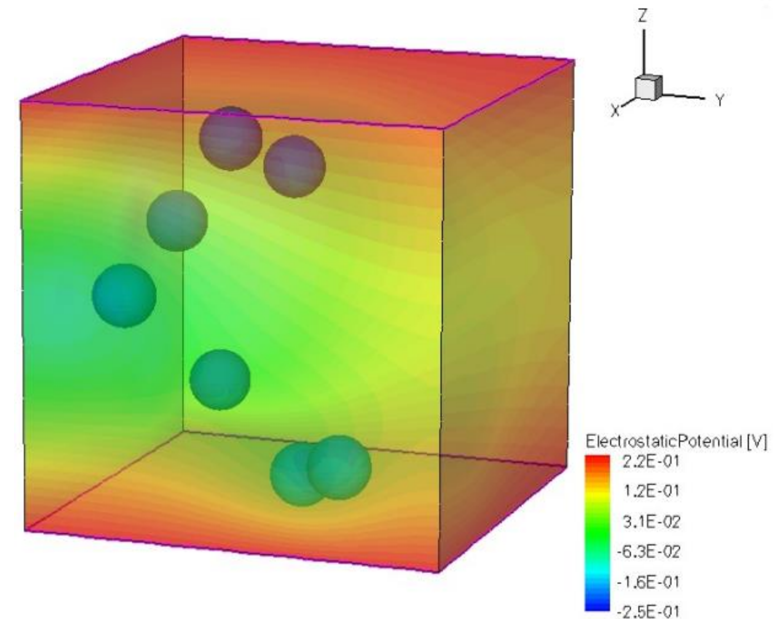
*Study of nano size defect clusters effect on macroscopic features of material.*

High energy particles bombardment creates damaged regions with trap levels:

1) Damaged region is treated as a spheric inclusion of different material with its own properties such as gap, effective mass, mobility, midgap states, etc.
2) According to literature, cluster dimensions ~20-100 nm, Concentration of traps within a cluster ~$10^{18}$ – $10^{20}$ $cm^{-3}$

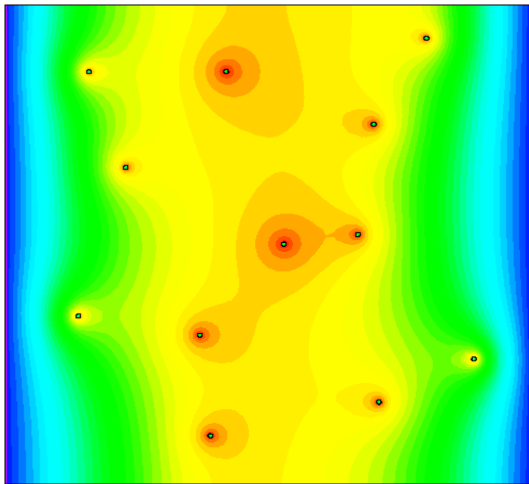
**Gossick model:** sphere shape cluster of acceptor type traps. Size of cluster 50 nm, acceptor energy levels $E_c$-0.55eV, concentration $10^{19}$ $cm^{-3}$.
Charge collected by traps creates potential, which is screened by conduction electrons.
Doping $N_d$ = $10^{12}$ $cm^{-3}$, screening radius 0.4 um.

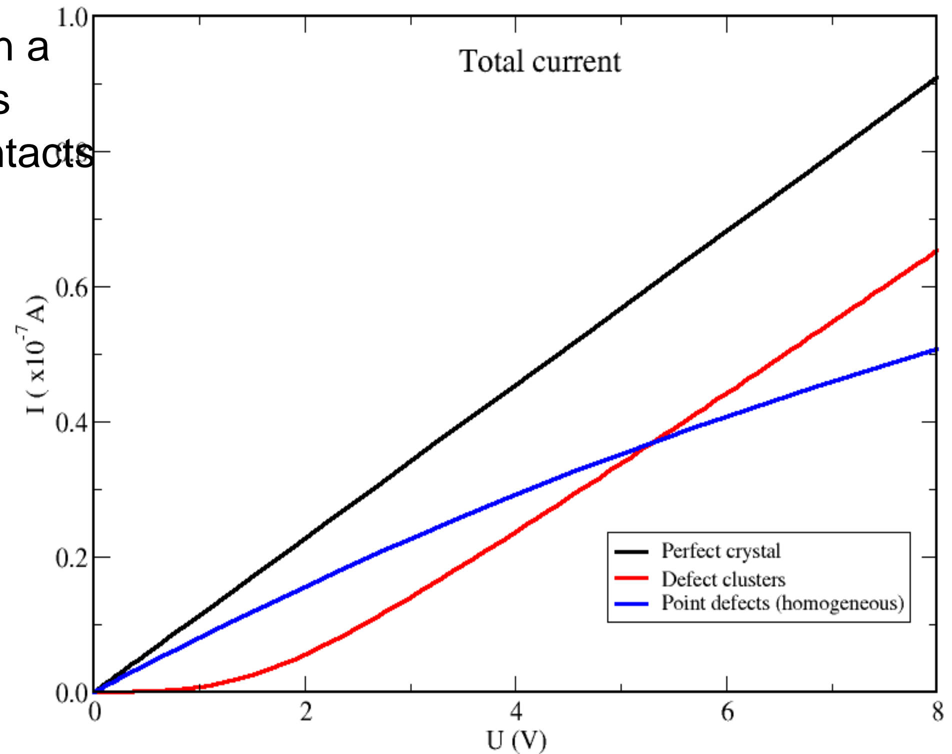


Voltamperic characteristics of clean Si sample, sample with defect clusters and sample with homogeneously distributed point defects

Electrostatic potential distribution within a sample with cluster defects with 0 Volts potential difference at left and right contacts (Synopsys INC. TCAD simulation).



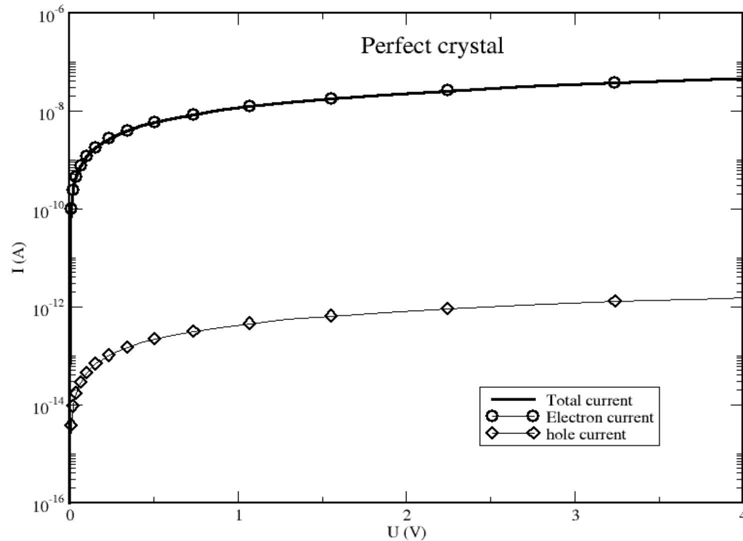


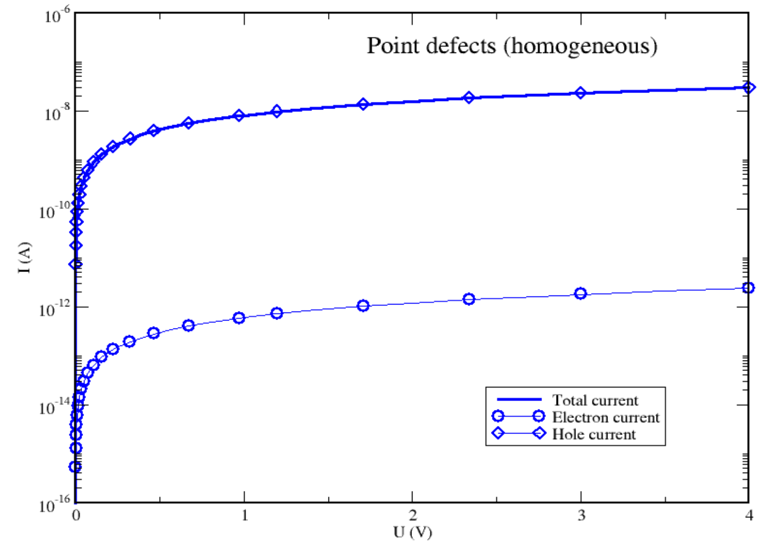

Sample with clusterized traps (red curve ) at high voltages reproduces I-V trend of pure crystal (black curve). All clusters at high voltages are screened and the sample acts as pure n-type semiconductor.

Below some critical external voltage screening remains too wide and cluster barriers too high for electrons to overcome resulting to decreased electron mobility.

If the same number of all traps were distributed homogeneously, with concentration:
(Number of clusters)* $10^{19}$ cm$^{-3}$ * pi* (50nm)$^2$ /(1um)$^2$ ~ $10^{15}$ cm$^{-3}$ >> Nd = $10^{12}$ cm$^{-3}$
then the sample would be of the p-type (blue line) with smaller conductivity than clean sample (black line).

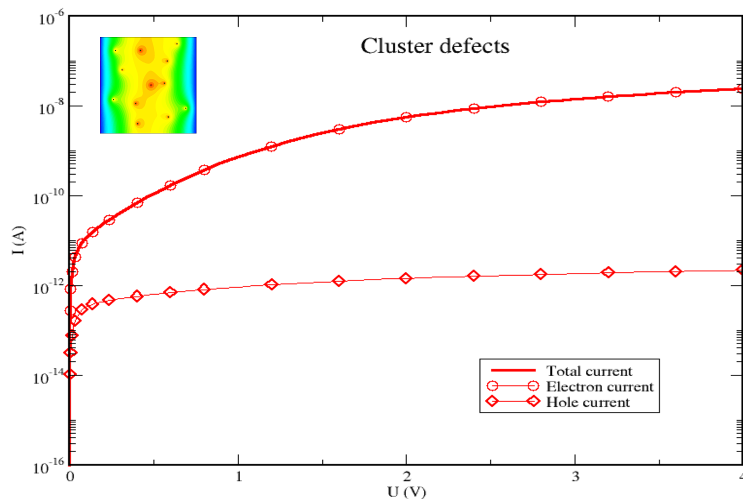
Total current components – electron and hole currents – compared in clean n-type silicon, silicon with point defects, and silicon with cluster defects



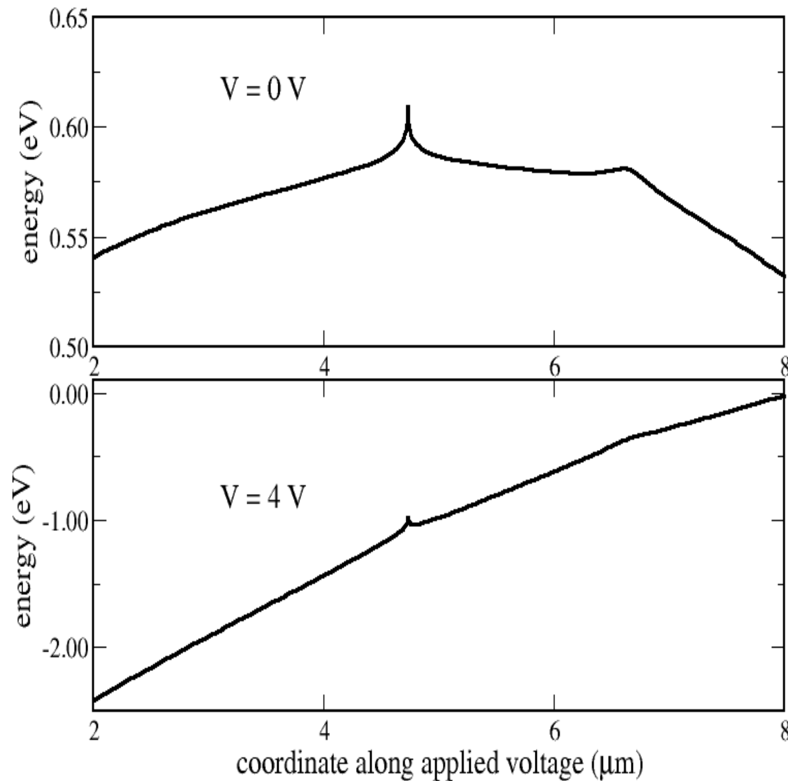

Homogeneously distributed point defects compensate donor doping and changes it into p-type silicon.
TRAP OCCUPANCY = 1

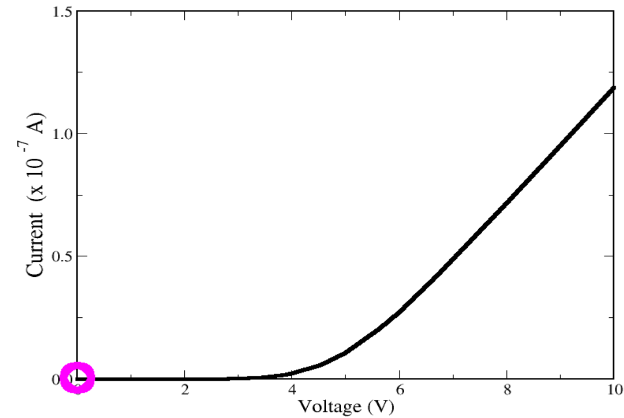
P- type silicon



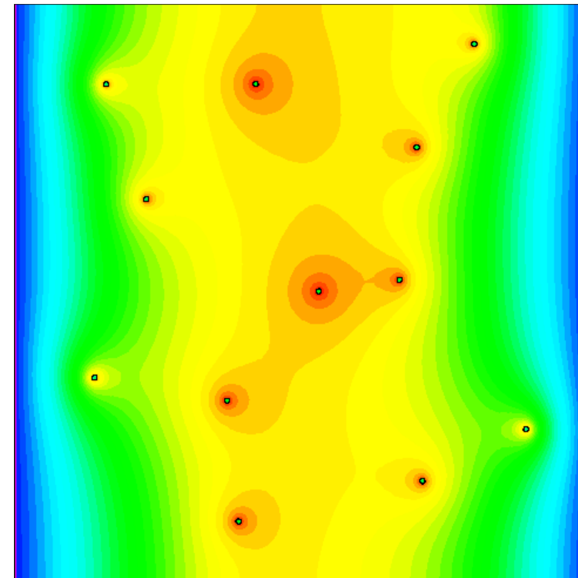

Same amount of point defects collected into clusters do not change the type of doping. The charge of trapped electrons forms electrostatic barrier around the cluster preventing further electron full trapping within the cluster.
TRAP OCCUPANCY ~0.3 – 0.8 !
Thus formed random electrostatic barriers significantly reduce charge carriers mobility.

Screening of cluster collected charge electric by external applied voltage field




Conduction band energy cuts along x-axis at 0 V and 4 V



Conduction band energy map evolution with increasing applied voltage along x-coordinate from 0 V to 10 V.

**This part of investigation was funded by Lithuanian Science Academy grant for CERN and Vilnius University collaboration (CERN-VU_02)**

# Fast Response detector based on GaN Schottky diode

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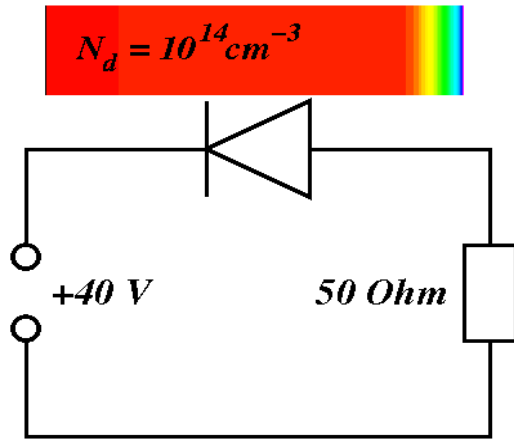
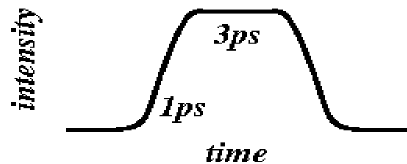
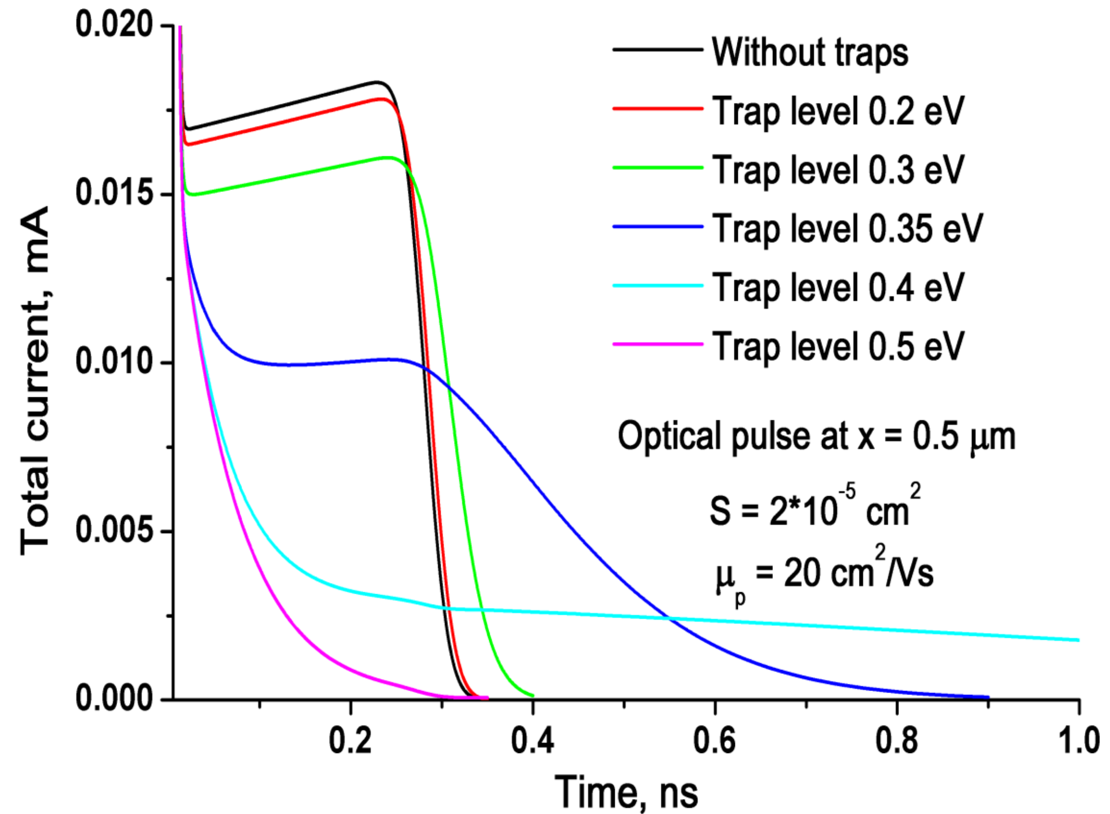
**Schottky diode (5 um)**

Potential distribution at zero voltage

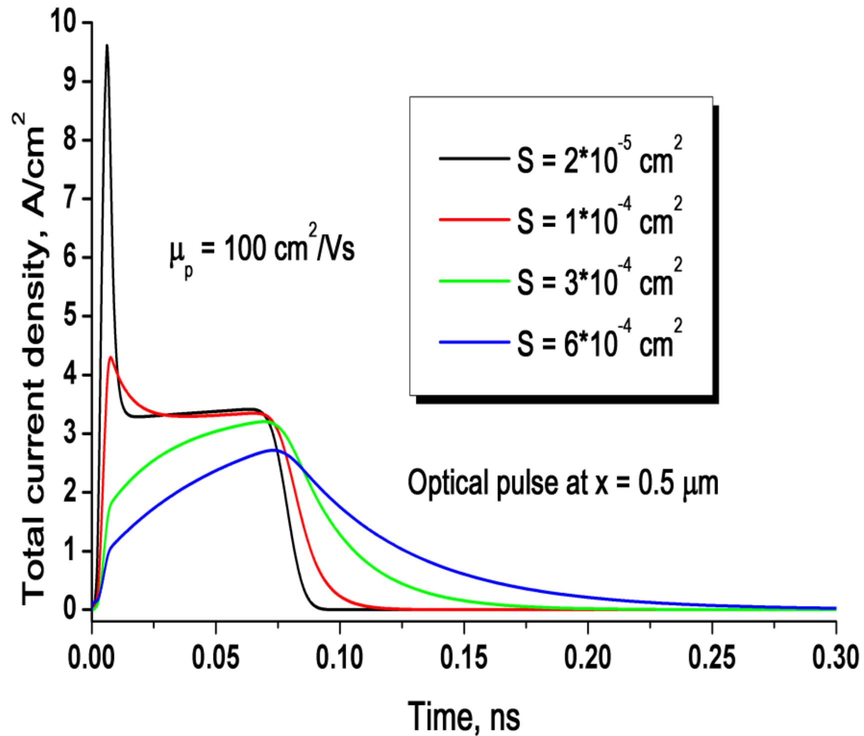


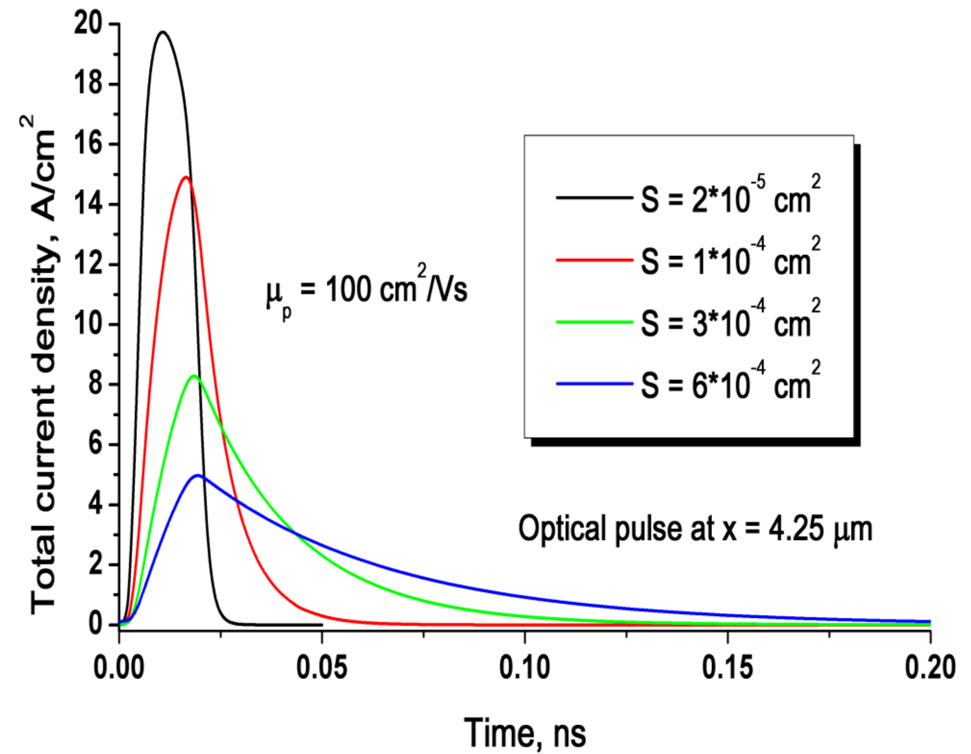




Shallow traps rapidly detrap and carrier drift is negligible. With increasing level depth detrapping slows and return to normal state takes time.

Capacitancy change of diode by increasing its width effects on response behaviour




Optically excited area far from Shottky barrier




Optically excitted area within the Shottky barrier region

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Thank You for Your Attention,

*Vilnius University team.*