TCAD simulation of Si crystal with different clusters.

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Simulation of defect cluster static states and free carrier trapping dynamics

- The TCAD Synopsis program was used for:
  - 1) investigation of electric field distribution in Si crystal containing different types and concentration of clusters;
  - 2) analysis of dynamics of electric field around the cluster during and after excitation by a short light pulse.
- An aim of presentation is an attraction of proposals to model the behavior of semiconductor in other situations.

Model equations (following Synopsys TCAD manual)

Poisson

$$\nabla \cdot (\varepsilon \nabla \phi + \vec{P}) = -q(p - n + N_{\mathrm{D}} - N_{\mathrm{A}}) - \rho_{\mathrm{trap}}$$

Continuity equations

$$\nabla \cdot \vec{J}_n = qR_{\mathrm{net}} + q\frac{\partial n}{\partial t} \qquad -\nabla \cdot \vec{J}_p = qR_{\mathrm{net}} + q\frac{\partial p}{\partial t}$$

Carrier transport (hydrodynamic model)

$$\vec{J}_n = q\mu_n\left(n\nabla E_{\mathrm{C}} + kT_n\nabla n - nkT_n\nabla \ln\gamma_n + \lambda_n f_n^{\mathrm{td}} kn\nabla T_n - 1.5nkT_n\nabla \ln m_n\right)$$

$$\vec{J}_p = q\mu_p\left(p\nabla E_{\mathrm{V}} - kT_p\nabla p + pkT_p\nabla \ln\gamma_p - \lambda_p f_p^{\mathrm{td}} kp\nabla T_p - 1.5pkT_p\nabla \ln m_p\right)$$

Fermi statistics for band electrons and holes

$$n = N_{\mathrm{C}} F_{1/2}\left(\frac{E_{\mathrm{F},n} - E_{\mathrm{C}}}{kT}\right) \qquad p = N_{\mathrm{V}} F_{1/2}\left(\frac{E_{\mathrm{V}} - E_{\mathrm{F},p}}{kT}\right)$$

Shokley-Read-Hall recombination, Doping dependent mobility,

Optical solver – Transfer Matrix Method (TMM), ***T = 300 K***

Trap description: Physics (material="cluster-Silicon"){

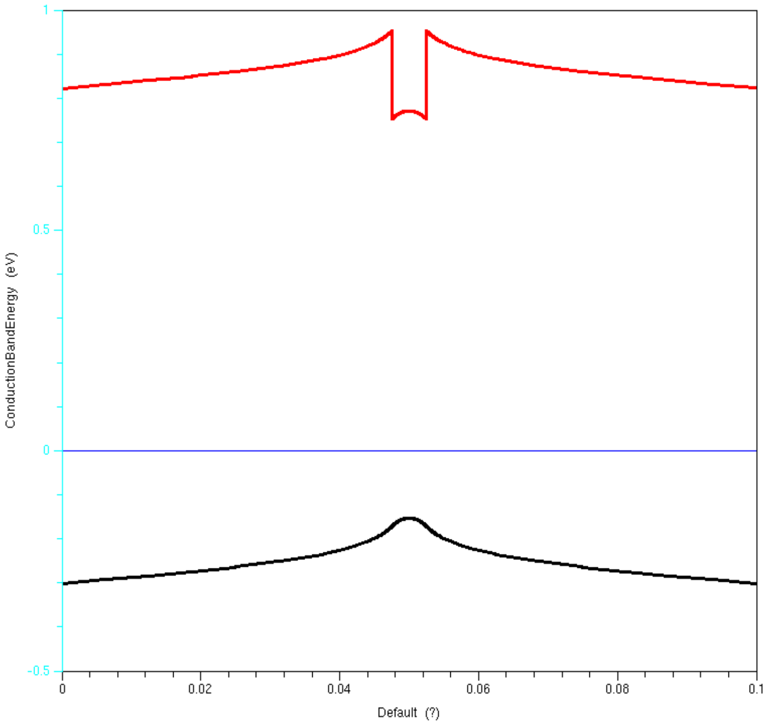
Traps(Acceptor Level EnergyMid=0.0 from Midgap eXsection=1e-15 hXsection=1e-15 Conc=1e19)

Study of trap clusters

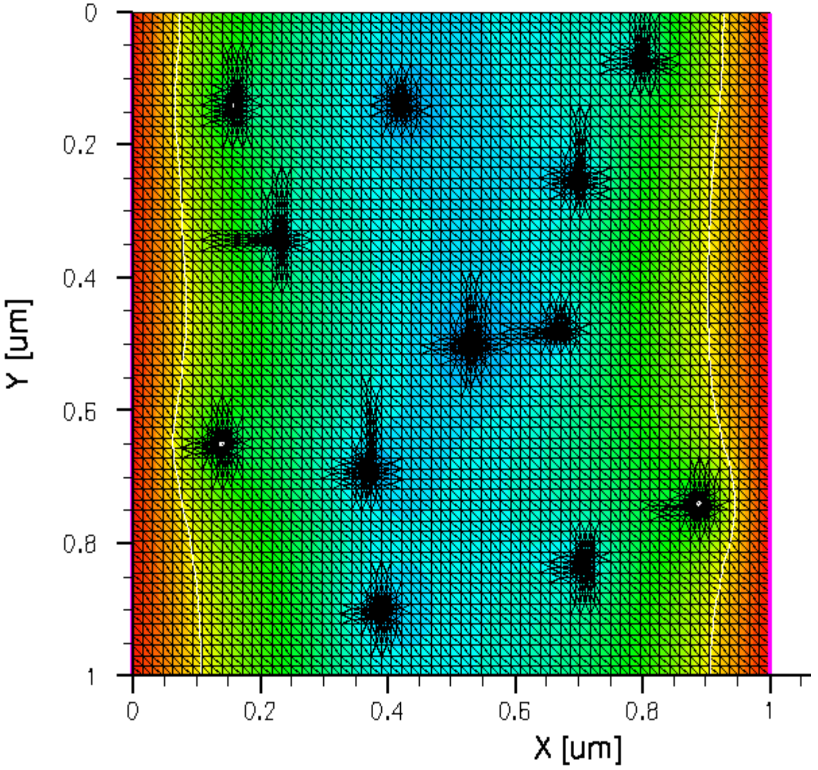
High energy particles bombardment creates damaged regions with trap levels:

1) Damaged region can be treated as a different material with its own properties such as gap, effective mass, mobility, etc.
2) According to literature, cluster dimensions ~20-100 nm, Concentration of traps within a cluster ~10^{19} – 10^{20} 1/cm^3

Gossick's model: Conduction and valence bands
Acceptor levels E_c-0.55eV, cluster size 50nm,
Overall doping N_d = 10^{12} 1/cm^3, screening radius 0.4 um.



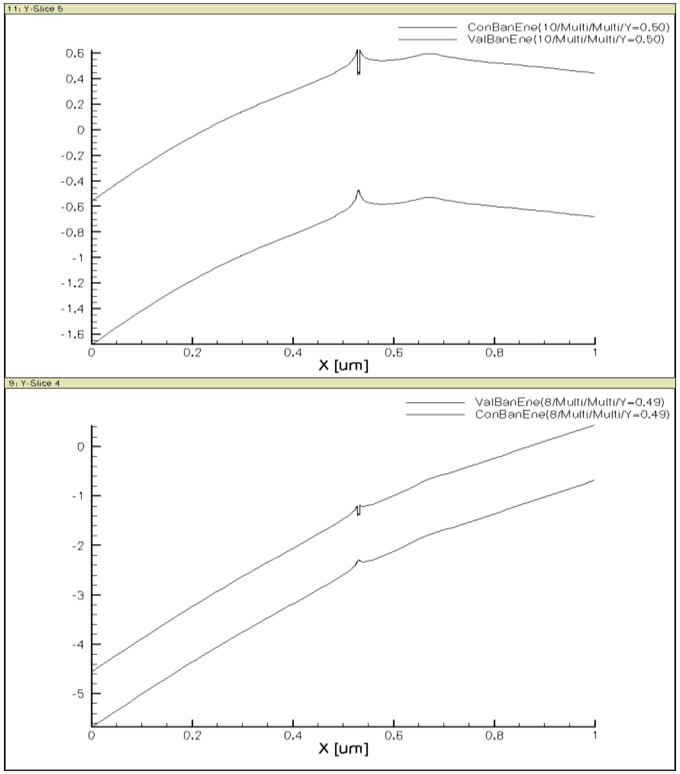
Electrostatic potential with boundary conditions 0 Volts at left and right contacts

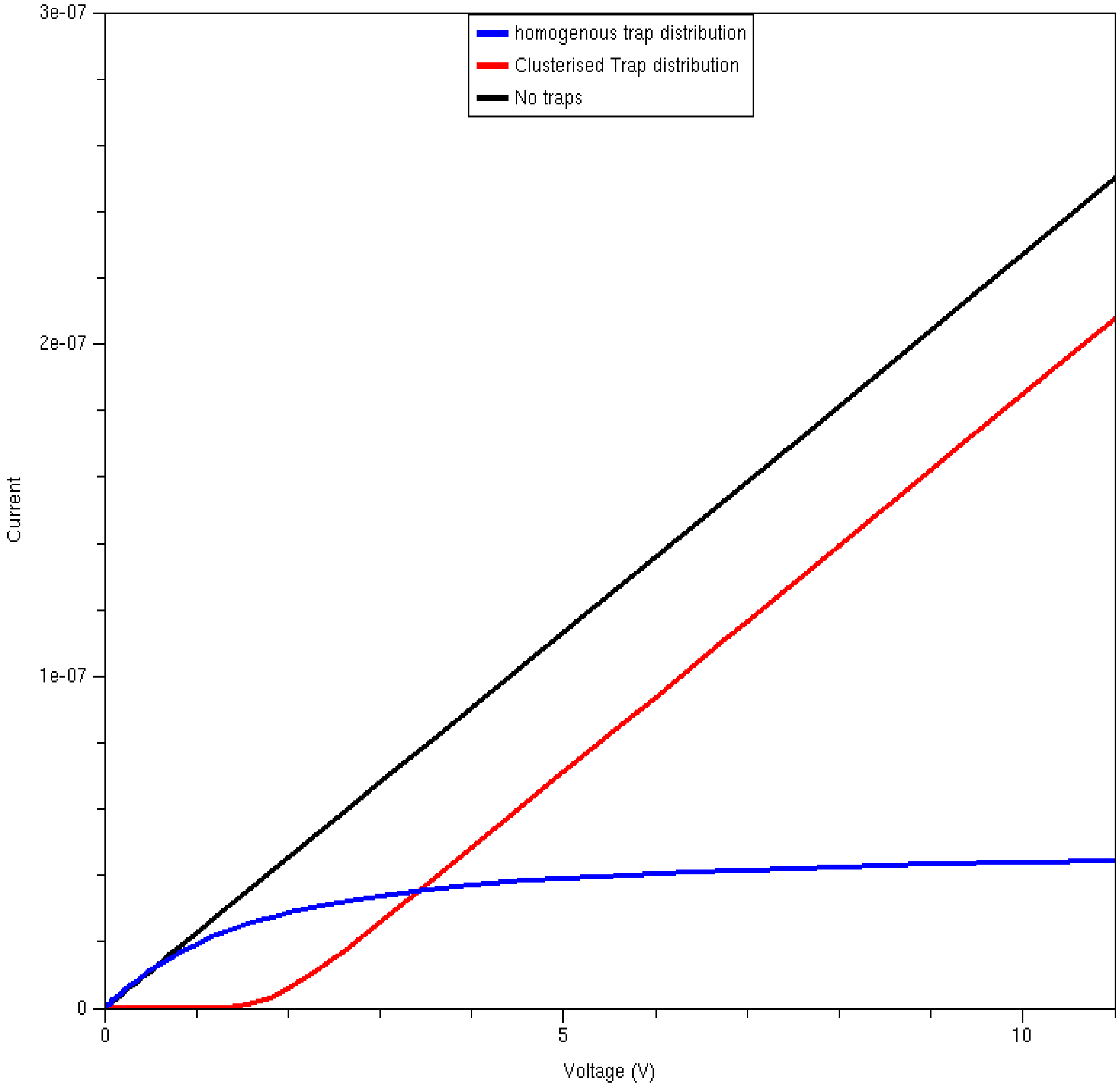


If all traps were distributed homogenously, with concentration: (Number of clusters)* 10^{19} 1/cm^3 * p_i* $(50nm)^2 /(1um)^2 \sim 10^{15}$ 1/cm^3 >> $N_d = 10^{12}$ 1/cm^3 , then the sample would be of the p-type (blue line) with less conductivity than a pure sample (black line).

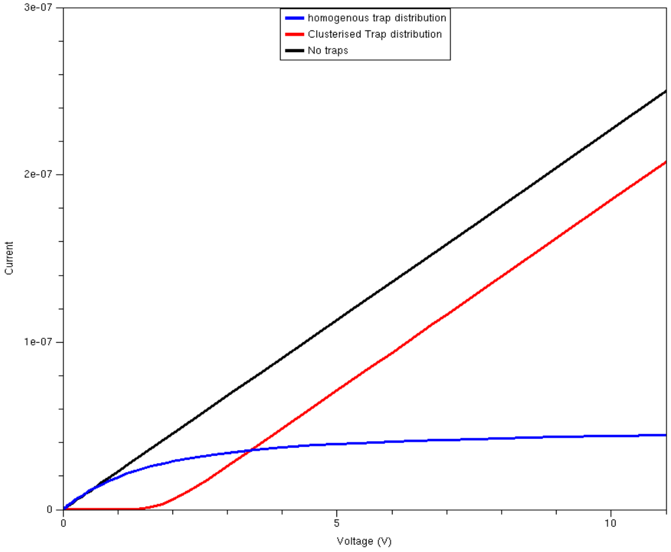
Sample with clusters remains of n-type in its main volume outside the cluster + cluster screen regions. Below some critical external voltage screening remains too wide and cluster barriers too high for electrons to overcome.

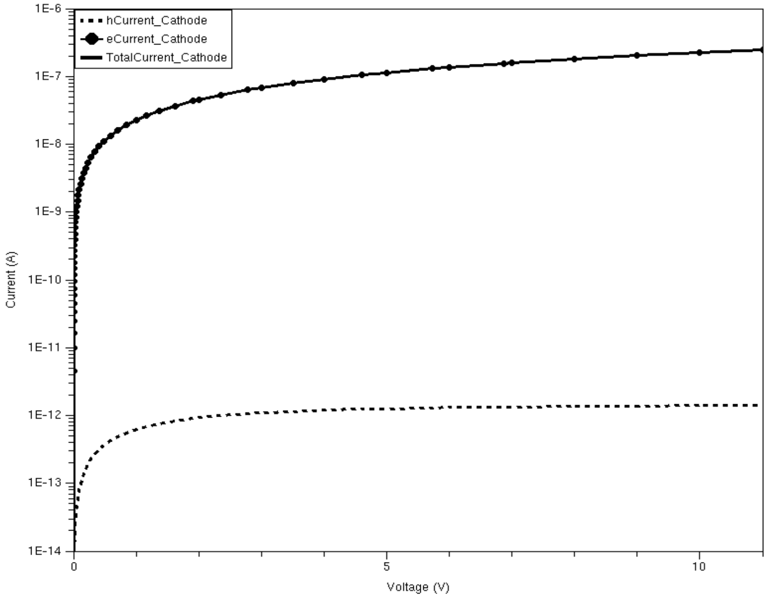
Band energies at 1 V and 5 V:

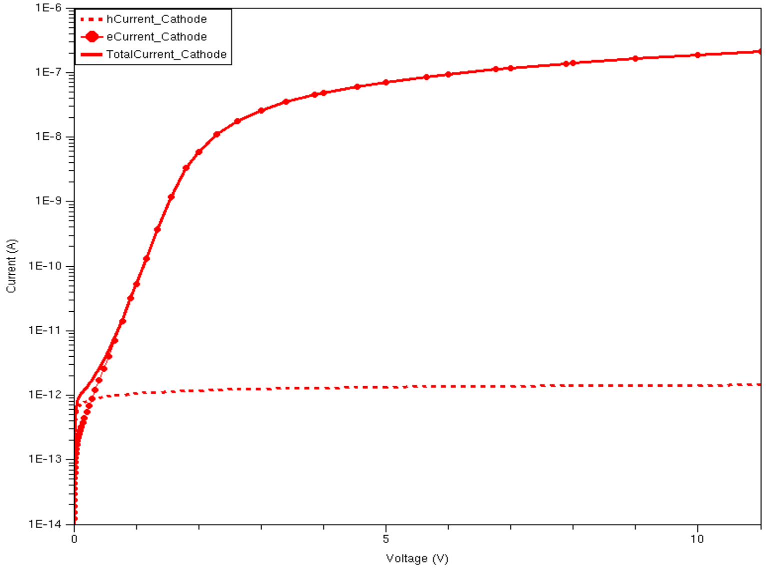


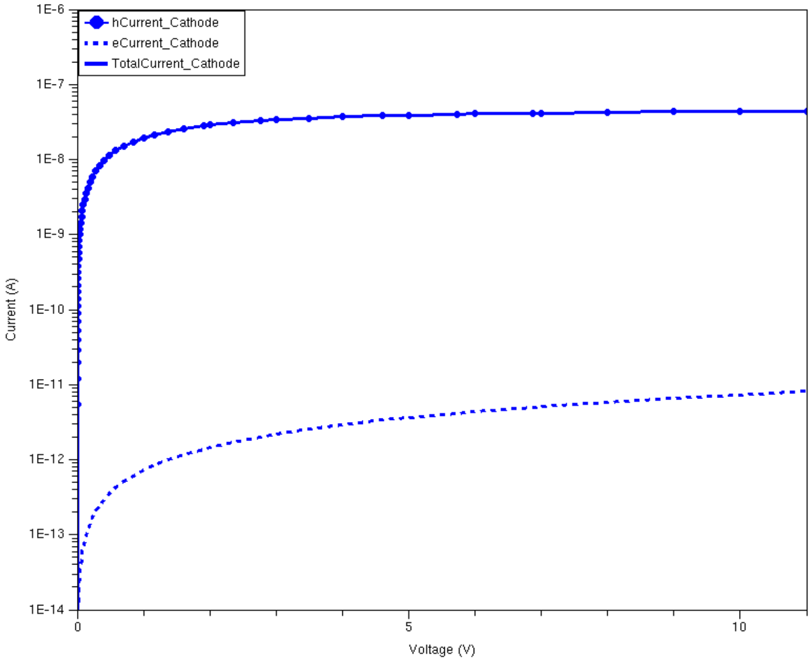


Current constituents for three cases

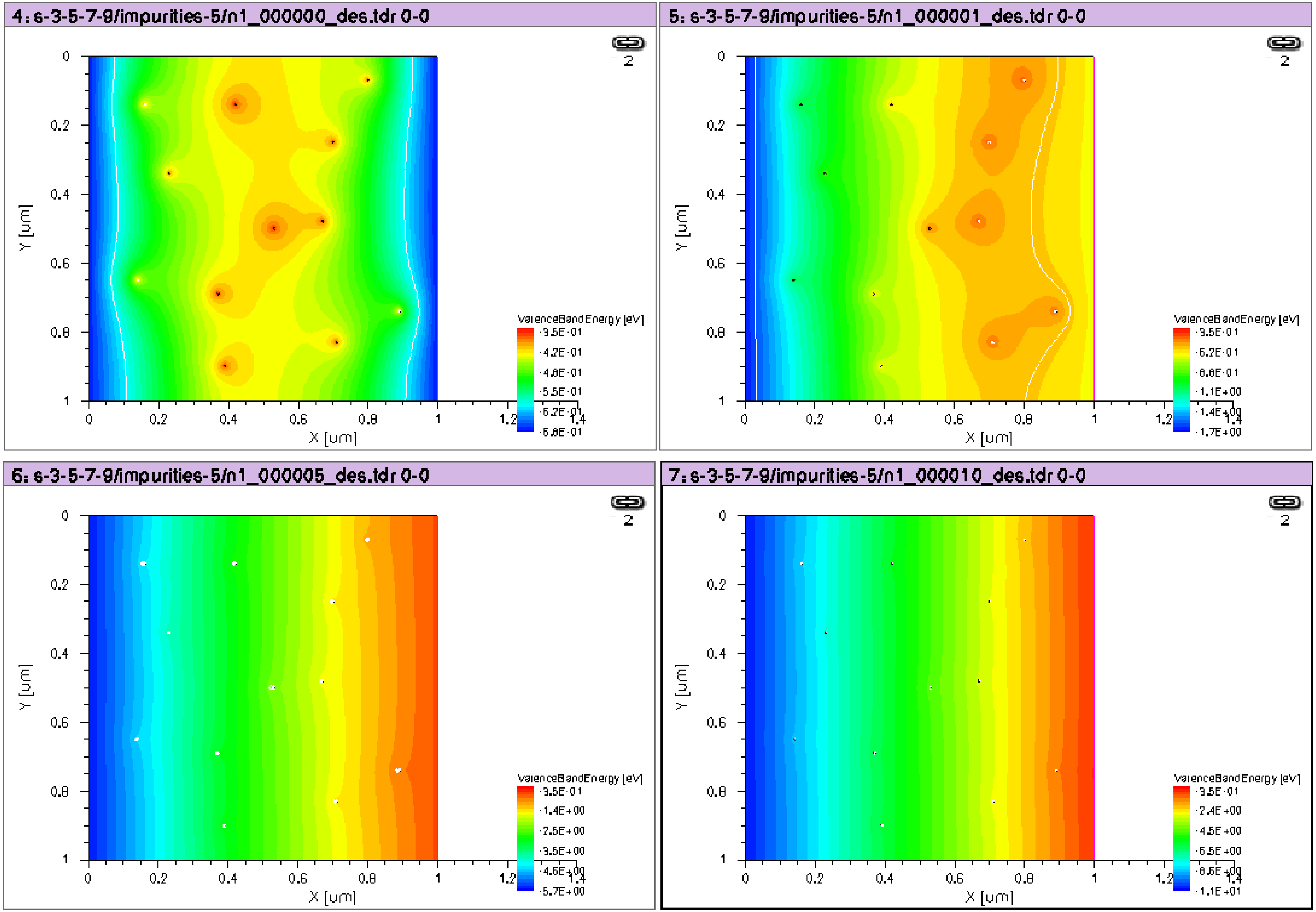



n-Si, no traps


n-Si, Clusterized trap distribution


n-Si, homogenous trap distribution

Hole dominating current in homogenous distribution case



Conduction band map at 0 V, 1 V, 5 V and 10 V.

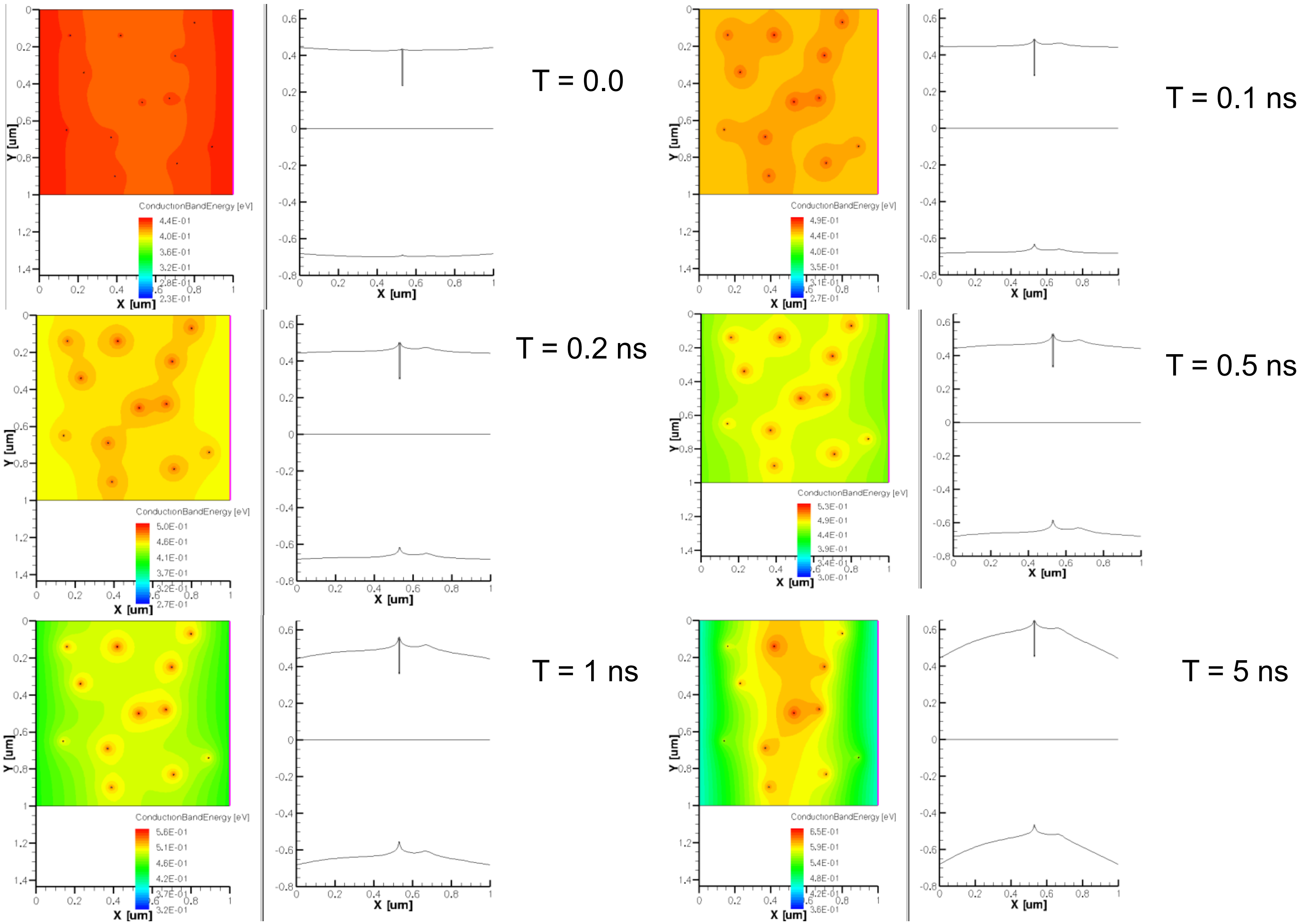
Free Carriers Trapping Dynamics in a Sample With Deffect Clusters (Extended Deffects)

The following experiment is simulated:

1) Sample is exposed to short light pulse (1 ns, 0.6um wavelength) excitation, free electrons and holes are generated.

2) Initially trap levels in the clusters are empty.

3) When light generation ends free electrons are attracted into clusters by traps. Time evolution of electron density and electrostatic potential (--> conduction and valence bands) is observed.



Conduction band map at various time steps

At t = 0 almost no screening of potential well. Free electrons are attracted into the cluster both by potential well and traps within the well.

In perspective the study will include:

1) a change the free carrier recombination and trapping terms in the TCAD program
2) averaging over large assemblies of parameters: cluster radius, density of clusters, trap density within a cluster, cluster inner material parameters, etc.
3) Analyse of the possible quantum effects:
   a) quantum well levels, if cluster size goes smaller:
      quantum level split ~ h^2/ma^2 ~0.07 eV at a = 10 nm
   b) ballistic transport – if cluster size goes biger (mean free path in Si ~ 500 nm)

Please to propose to model the behavior of semiconductor in other situations!

THANK YOU FOR YOUR ATTENTION !