Development of the space oriented vacancy – interstitial cluster model

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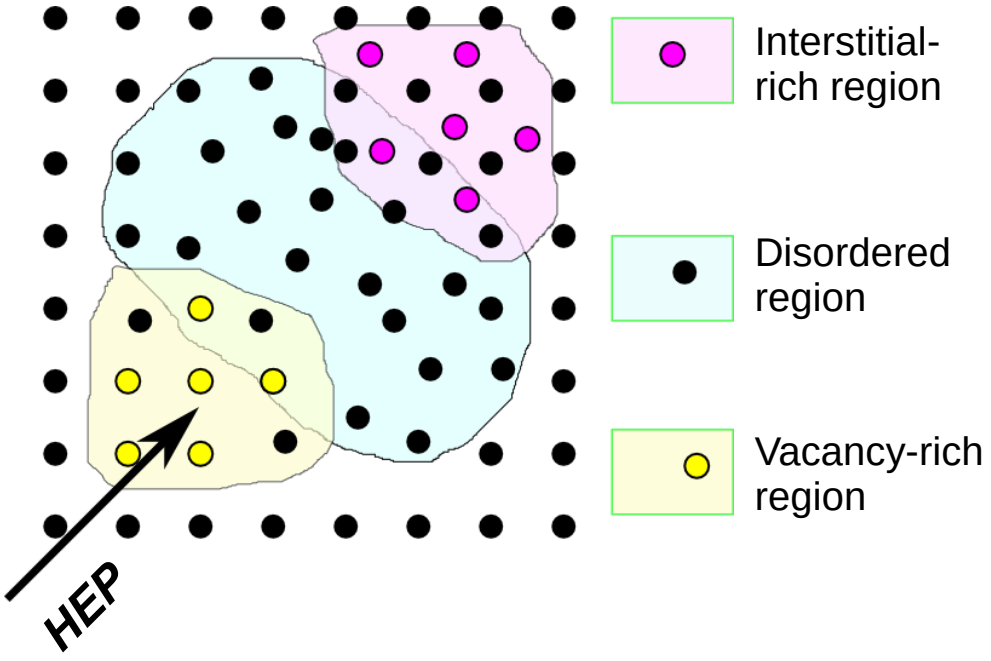
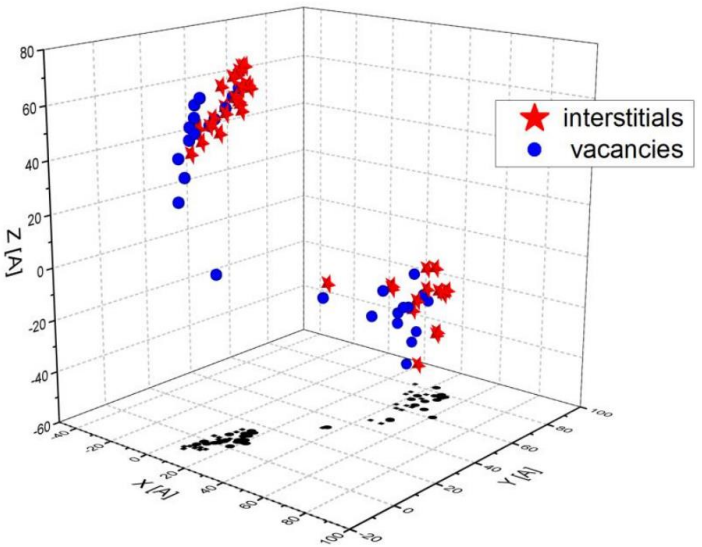
Vacancy – Interstitial Defect Cluster Model Updated

Updated model:

High Energy Particle (HEP) destroys the lattice:





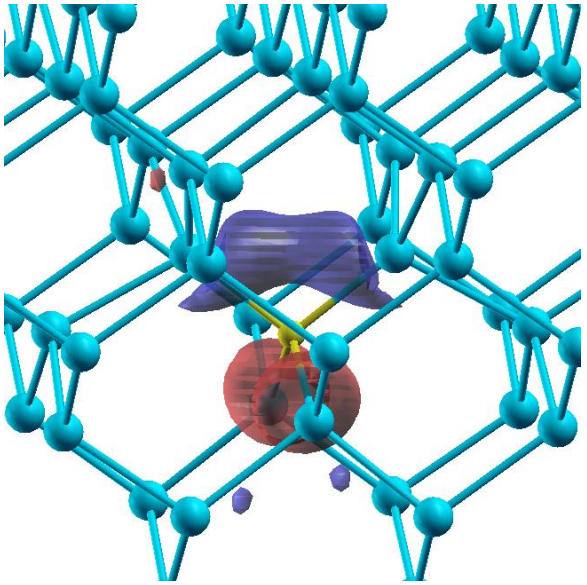
36 V/I after recombination (20%)

TRIM and TCAS simulation results, presented by G. Lindstroem, 24th RD50 workshop, Bucharest, 2014.

After relaxation of cascade deffect and recombination of I-V pairs the rest of the vacancies and interstitials remain separated in space.

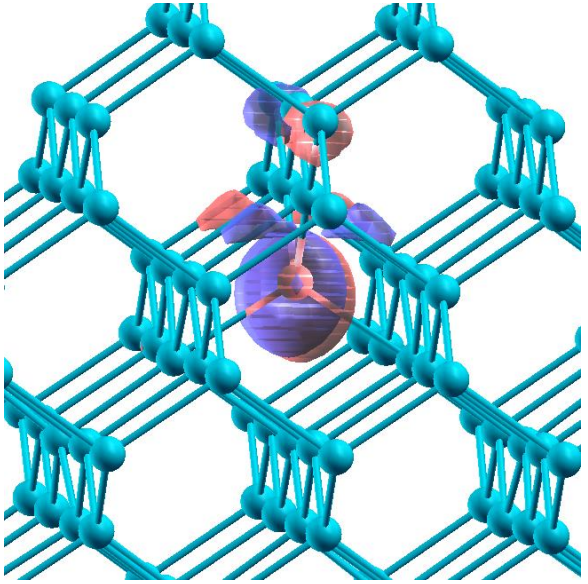
In earlier model, presented in 24th RD50 workshop, Bucharest, 2014 by E. Zasinas, only disordered region was considered.

Vacancy and Interstitial defect



Vacancy defect, Td symmetry.
Wave function of a localized electron
in the acceptor site.

Neutral vacancy defect is known to be of
the **acceptor** type.



Interstitial defect, Td symmetry.
Wave function of a localized hole
in the donor site.

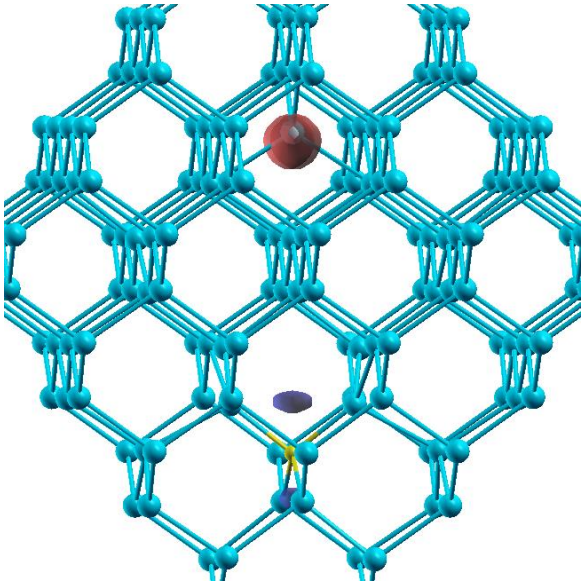
Interstitial defect in Td symmetry state is known
to be of the **donor** type (Ec – 0.39 eV)
Mukashev et al, Jpn. J. Appl. Phys. 21, 399 (1982).

Here and below: Density functional calculations with ORCA program. Calculation details: R-I approximation, exchange-correlation potential BP86, basis of wave functions SVP and SV/J. See ORCA manual.
Red and blue colors of wave function isosurfaces stand for the different sign of wave function.

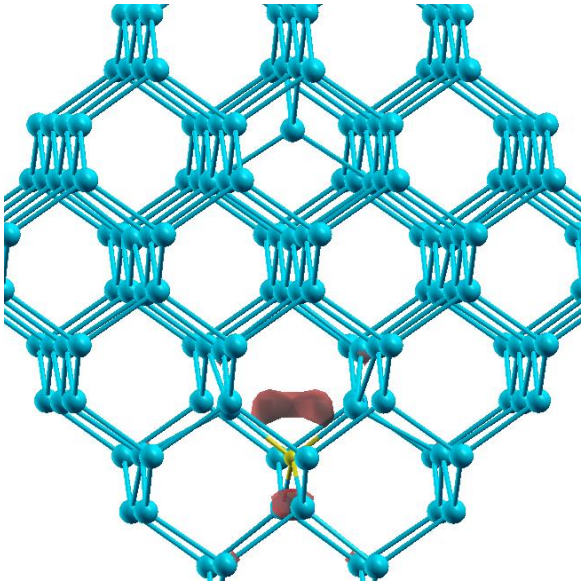
Vacancy – Interstitial pair (Frenkel pair) defect

When vacancy and interstitial are approached to each other to form a pair then the extra electrons given by interstitial are “pumped” away from the interstitial site to the vacancy site. (Like in a ionic type molecule or crystal electrons mainly are located nearby more electronegative ion.)

! Interstitial and vacancy exchange their roles:
Interstitial turns into **acceptor** and vacancy into **donor**:



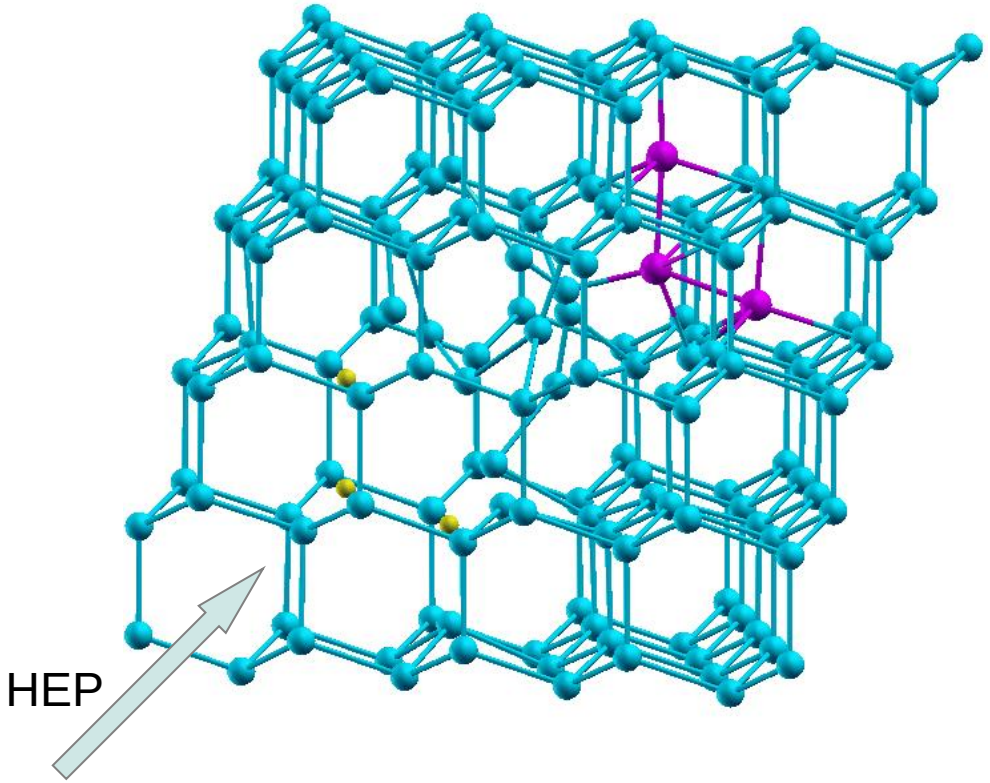
Charged (-) system, one electron added.
The **electron** wave function (~80% of it) is located nearby interstitial site (or the electron is accepted by interstitial site).



Charged (+) system, one electron removed.
The **hole** wave function is located nearby vacancy site (or the electron is donated away by vacancy site).

The same is expected to take place in cluster.

Vacancy – Interstitial defect cluster

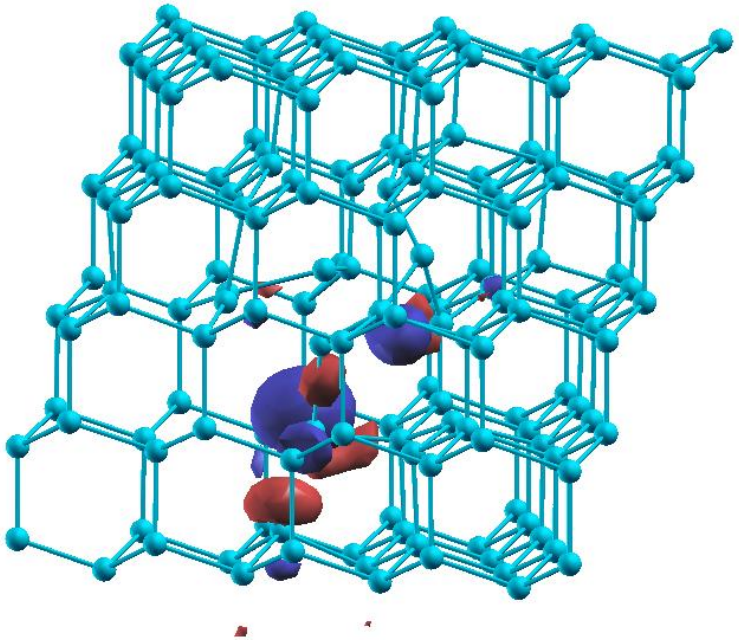


Initial structure imitating crystal structure damage by the High Energy Particle (HEP):

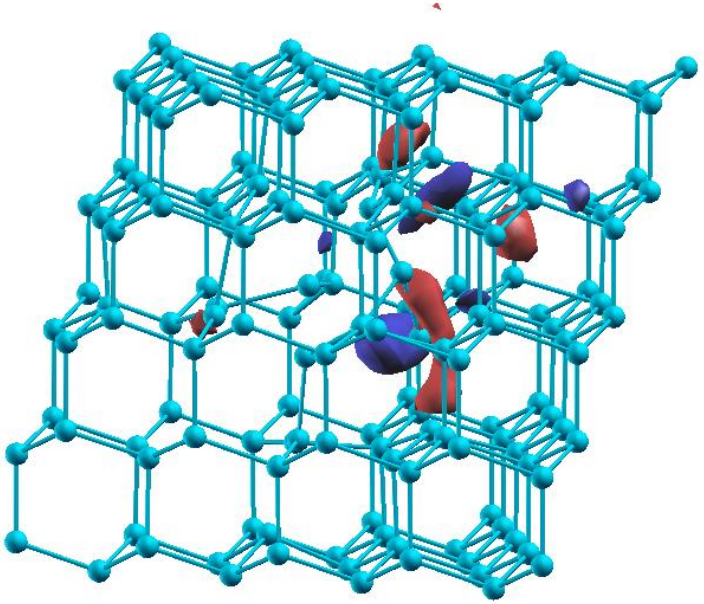
yellow are vacancy sites
magenta – interstitial Si.

Vacancy – Interstitial defect cluster relaxation

Partially relaxed defect structure:



Wave function of located hole.
Holes locate closer to vacancy-rich region.
I.e. Electrons are removed from this region,
vacancy rich region plays a role of donor.

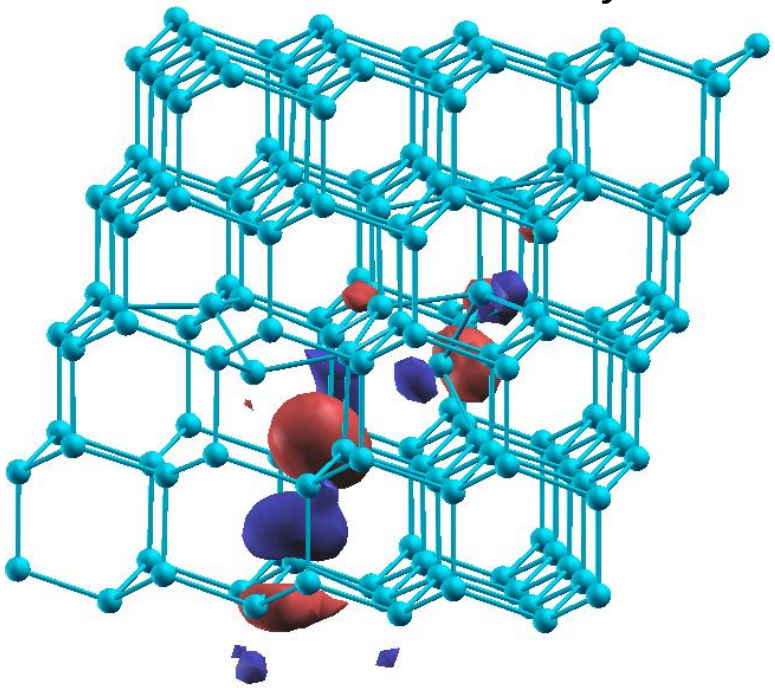


Wave function of located electron.
Electrons locate closer to interstitial-rich region.
I.e. interstitial rich region plays a role of acceptor.

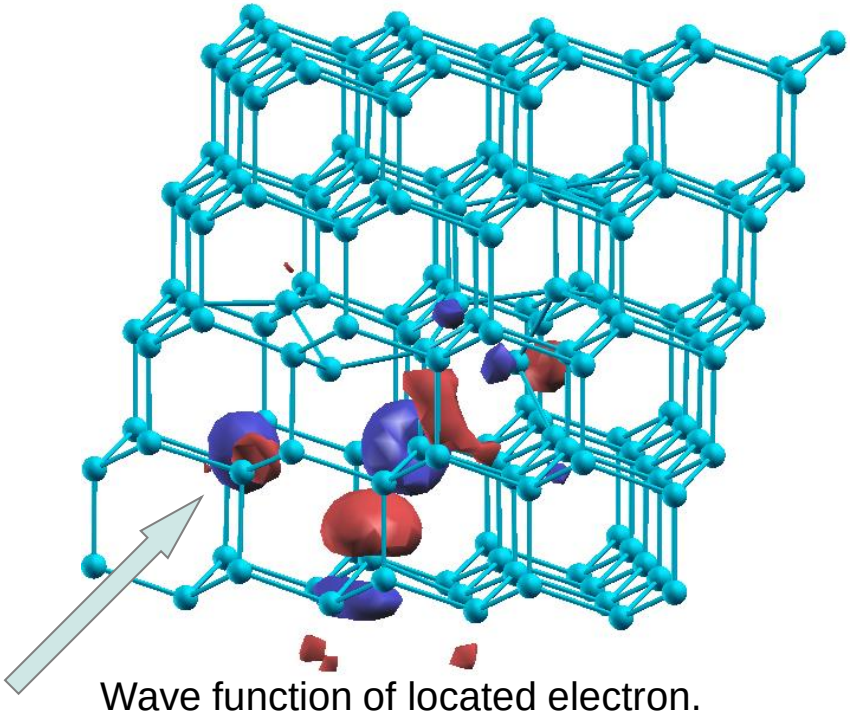
Situation is similar to the single I-V pair case.

Vacancy – Interstitial defect cluster relaxation

Fully relaxed defect structure:



Wave function of located hole.

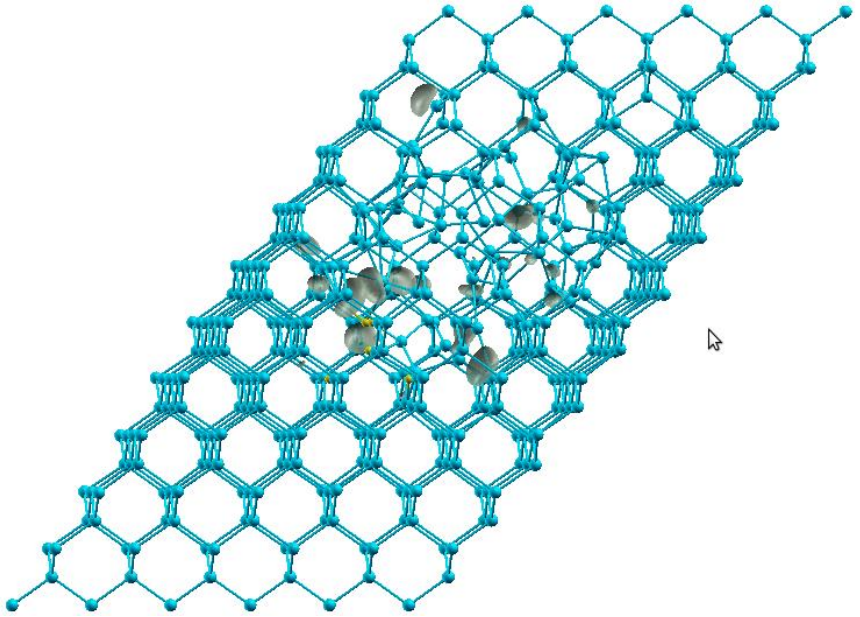


Wave function of located electron.
Part of wave function is located in vacancy region (shown by arrow).

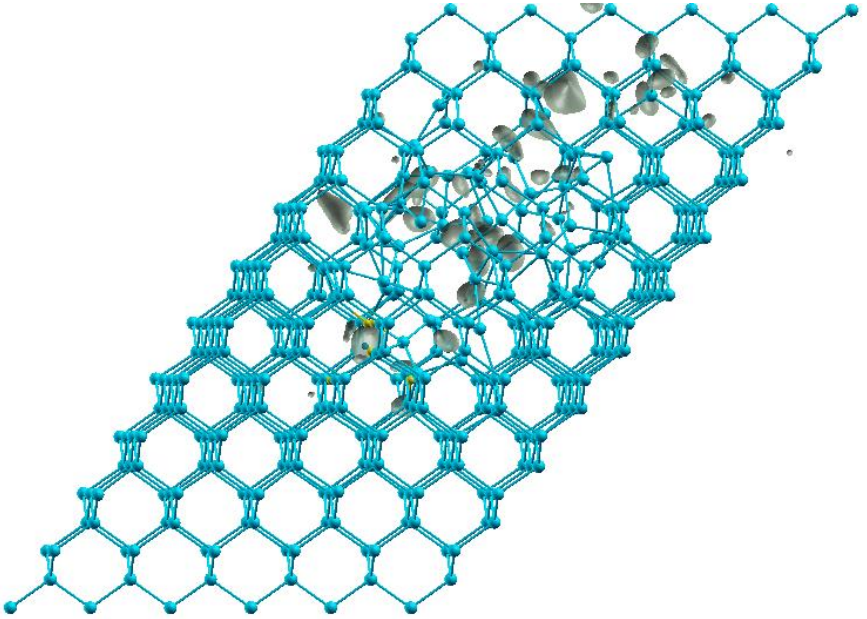
Situation for the fully relaxed structure differs from the single I-V pair case:

- hole and donor state wave functions are located within the same area
- Interstitionals entered into covalent bonds with the lattice ions and lost their abilities to localize holes or electrons.
- Vacancies partially restored their properties of acceptor type defect.

Recent calculation of the bigger cluster:
432 atoms, 50 atoms in disordered positions. 5 separated apart V-I (Frenkel) pairs



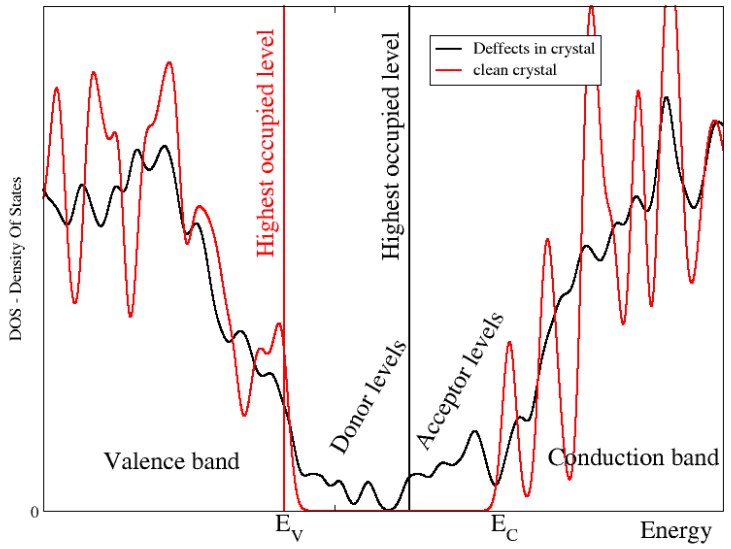
One of Donor states wave function isosurface at 0.25 of its maximum value. The wave function main weight is closer to the region with vacancies (yellow balls).



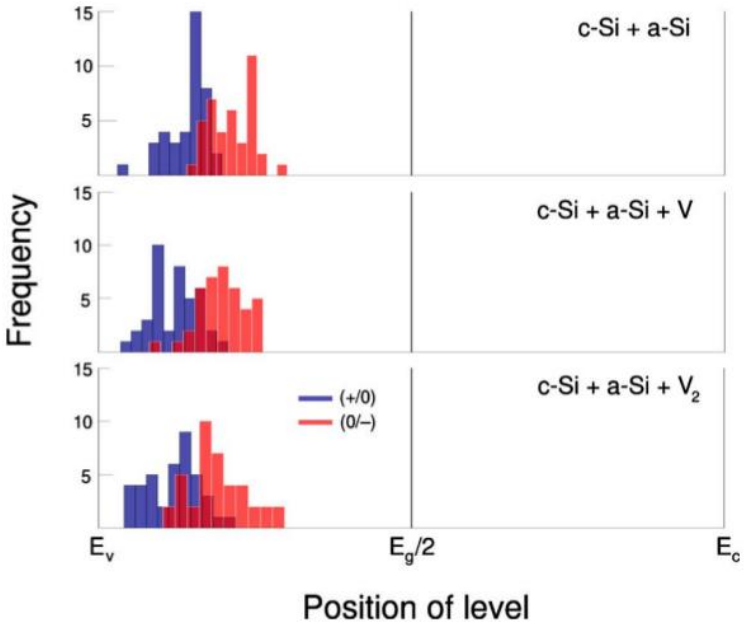
One of Acceptor states wave function isosurface at 0.25 of its maximum value. The wave function main weight is closer to the region with interstitials.

Density functional calculations with ABINIT software.

Density of states in the Vacancy – Interstitial defect cluster



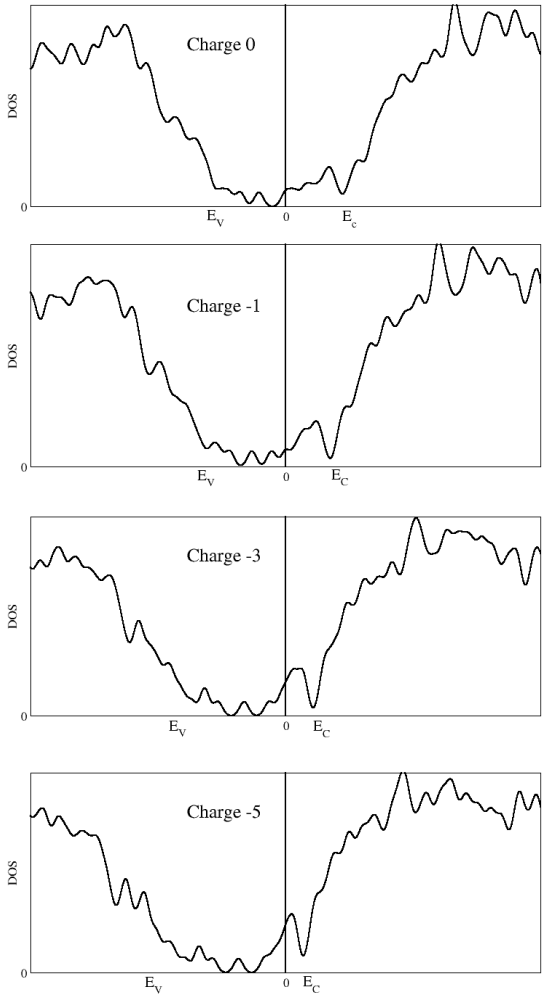
Density of states and fermi level for the defect cluster (black) compared with the same quantities of the clean Si crystal (red)



E. Holmstrom et al, Phys. Rev. B, **82**, 104111 (2010). DFT calculations. Statistical distribution of the highest energy donor state and the lowest energy acceptor state levels.

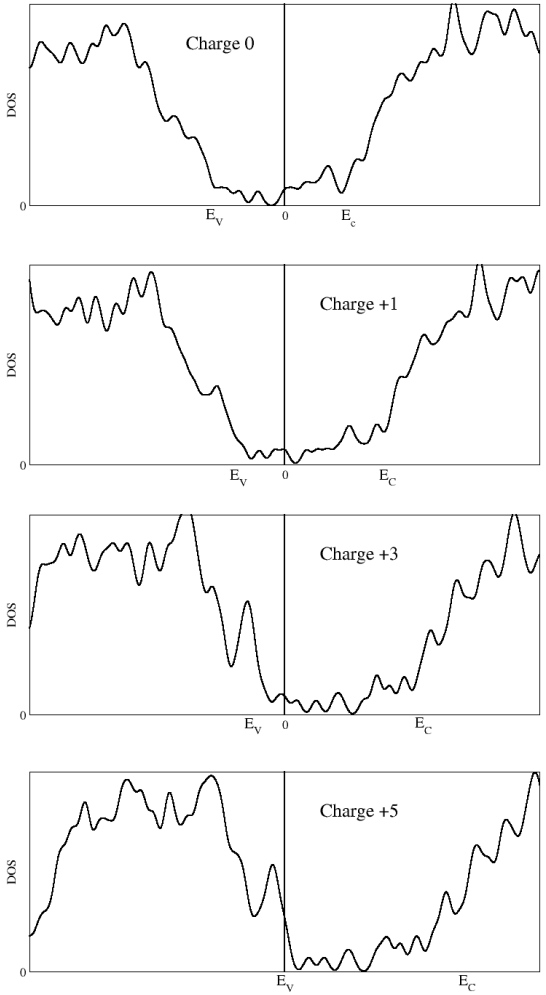
DOS of charged Vacancy – Interstitial defect cluster

Last year (2014 Bucharest) question to us: How much charge the cluster can accept? One way to answer it is to calculate the charged system and find at which charge the fermi level touches valence or conduction band.



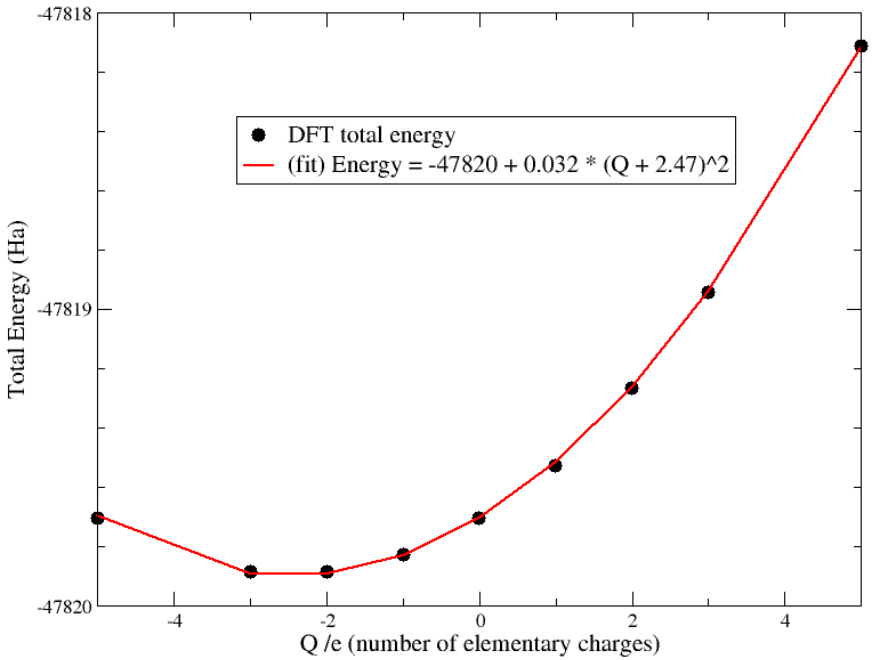
Adding electrons

As far as we can see from the results presented here cluster may accept up to five holes and more than five (may be up to seven) electrons.
Taking 1 - 5 elementary charges per ~10 Angstrom diameter sphere one gets
~(0.2 - 1)10^{22} cm^{-3}
localized charge concentration.

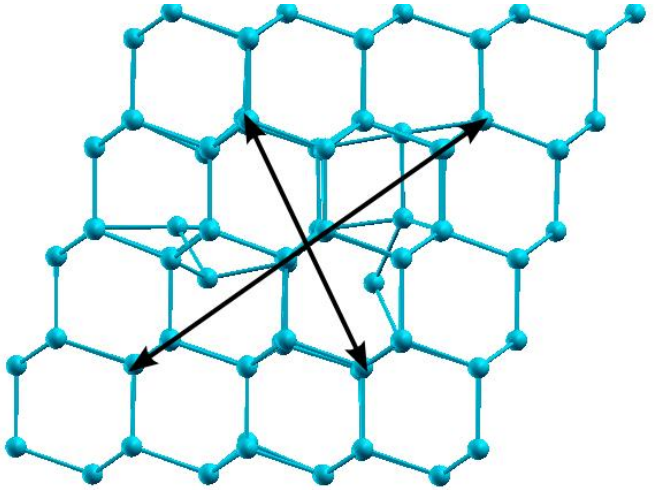


Removing electrons

Charging energy of Vacancy – Interstitial defect cluster



Total energy versus charge



Distances of 8.14 and 12.54 Angstroms shown by arrow segments are the typical dimensions of cluster.

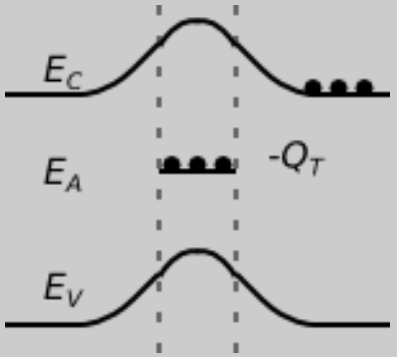
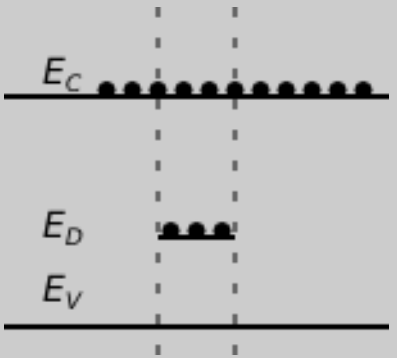
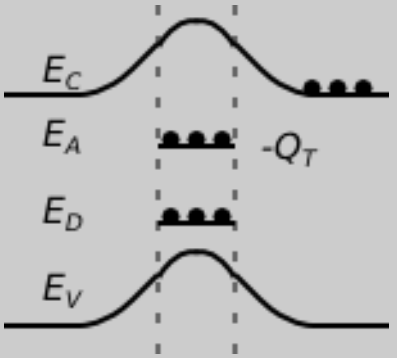
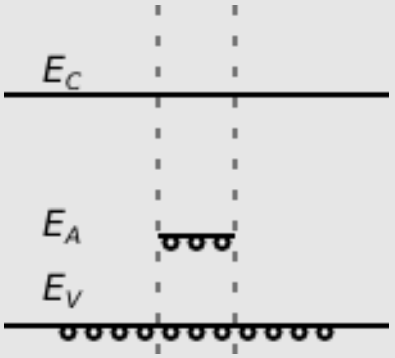
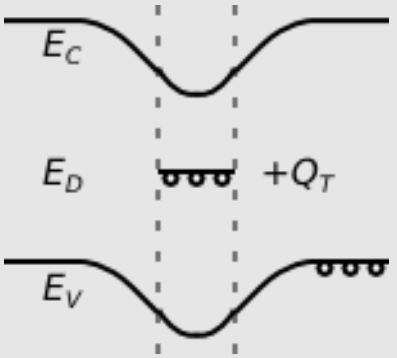
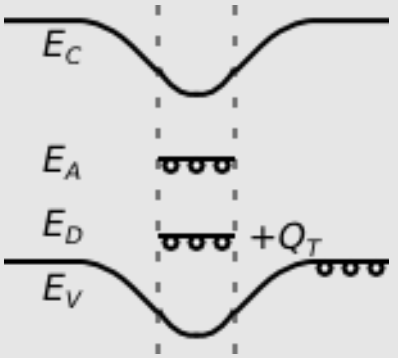
Energy dependence on charge is well fitted with capacitor formula:

$$E = E_0 + \frac{(q - q_0)^2}{2C}$$

with q_0 = -2.47 e and C = 7.8 Angstroms (8.7 10^{-20} F).
Such a value of capacitance fits well with the size of our studied cluster.
This particular cluster configuration appears to have the minimal energy when charged with -2e or -3e.

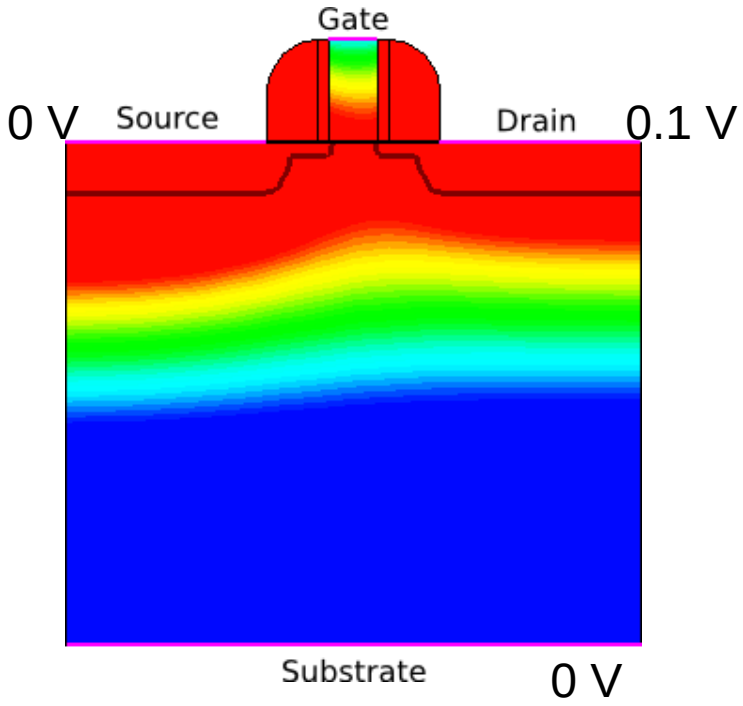
Multiple state defect clusters effect on Field-Effect Transistor (FET) voltamperic characteristics

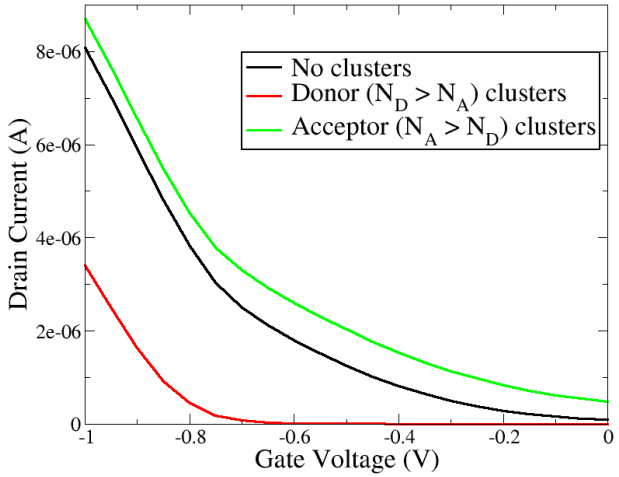
Gossick model of the defect cluster

	Acceptor traps	*Donor traps*	*Both types of traps*
n - doped			
p - doped			

Band structure in and around the core of the cluster

Clean (without clusters) FET voltamperic characteristic





Two dimensional FET model taken from TCAD example library.

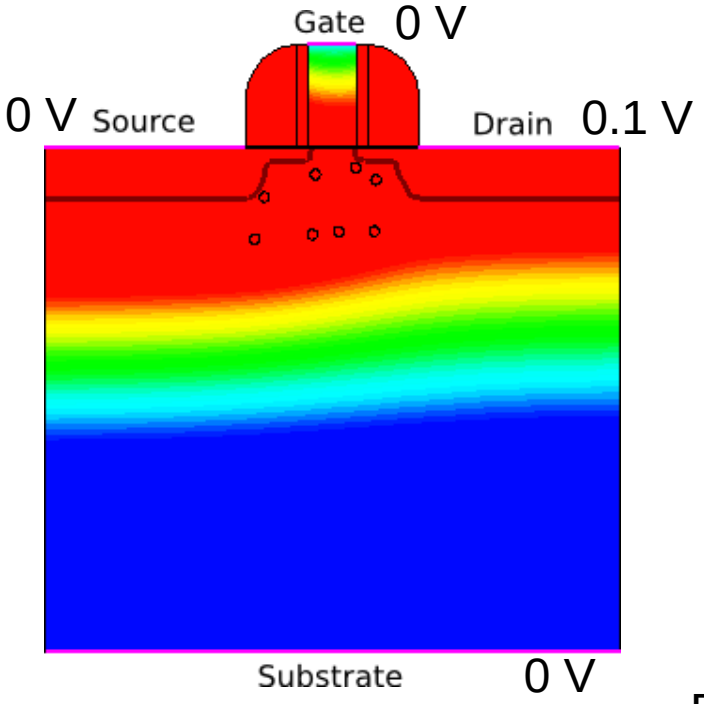
model details:
p-n-p type, doping concentrations
Substrate: $n = 10^{15}$ cm^{-3},
Source and Drain subcontact $p+ = 10^{17}$ cm^{-3}.

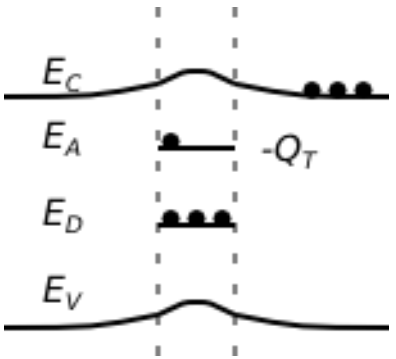
At first Substrate, Source, and Gate contacts are fixed at 0.0 Volts and Drain contact voltage is ramped up to 0.1 Volts and fixed at this value.

Then negative voltage is applied to the Gate contact and the total current through the Drain contact is measured.

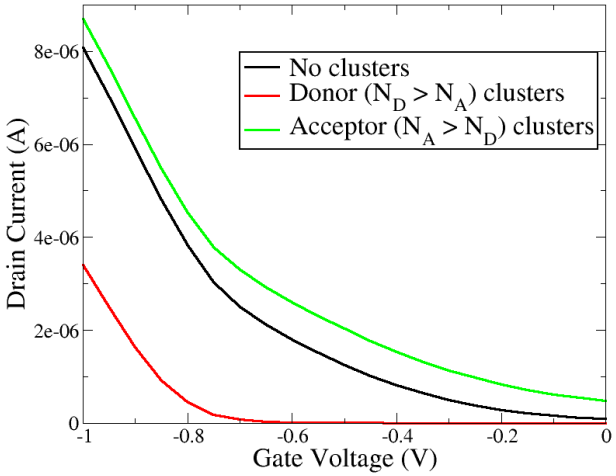
Resulting $I_{Drain} – V_{Gate}$ dependence is shown as a black curve in the graph at left.

FET with acceptor states rich clusters





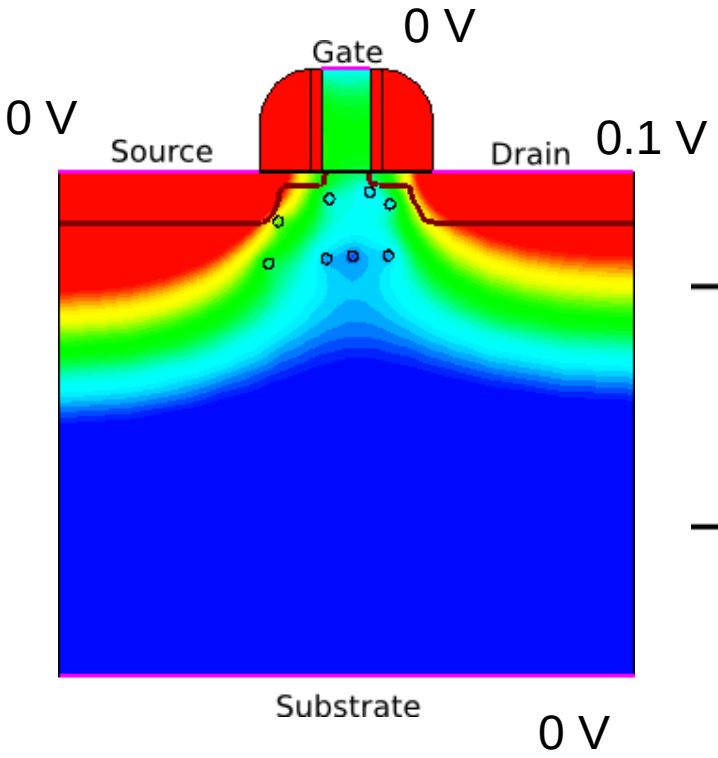
Cluster with dominating acceptor states within its core. And very little or now donor states inside:
$N_D << N_A$.
$E_A = E_C - 0.65$ eV, $N_A = 10^{17}$-10^{19} cm^{-3}
$E_D = E_C - 0.85$ eV, $N_D = 10^{15}$ cm^{-3}.
All cross-sections 10^{-15} cm^2.
Cluster radius 0.001 um.

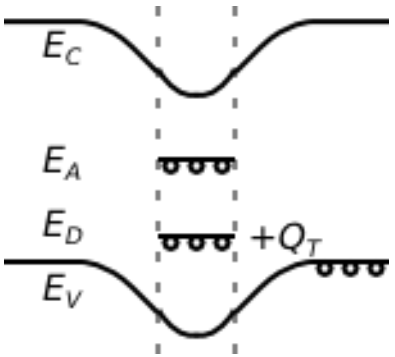


For the given doping and traps parameters the typical acceptor trap occupation is ~0.001-0.01 (0.1 – 1 % of traps are filled with electrons). Very small charge is located in the clusters and its potential is negligible.

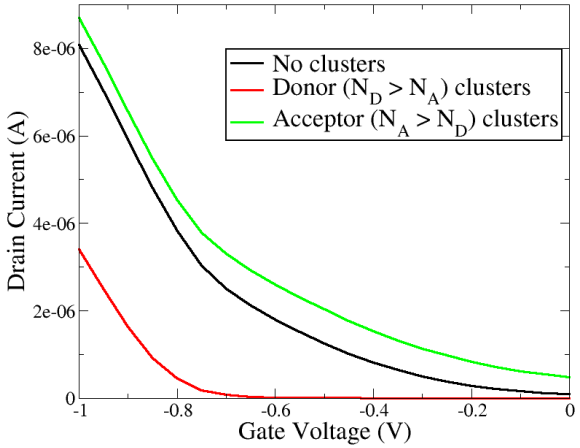
In this case cluster acceptor states act as compensation centers: they reduce concentration of the doped free electrons. As a result of the law of the mass action ($np = n_i^2$) concentration of free holes increases leading to the current increase – green curve in the graph at left.

FET with multiple states clusters





Cluster with both types of states - donor and acceptor - within its core.
$N_D \sim N_A$ and $N_D > N_A$.
$E_A = E_C - 0.65$ eV, $N_A = 10^{17}$ cm^{-3}
$E_D = E_C - 0.85$ eV, $N_D = 10^{17}$-10^{19} cm^{-3}.
All cross-sections 10^{-15} cm^2.
Cluster radius 0.001 um.



For the given parameters typical donor trap occupations are ~0.05-0.1. The potential induced by trapped holes is not as negligible as in previous case. Two factors lead to significant decrease of current (red curve at left):

- decrease of free holes,
- fluctuating potential obstacles preventing hole transport.

Thank You for your attention.

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