Modelling of Radiation Induced Vacancy-Interstitial Clusters

Ernestas Žąsinas & Juozas Vaitkus

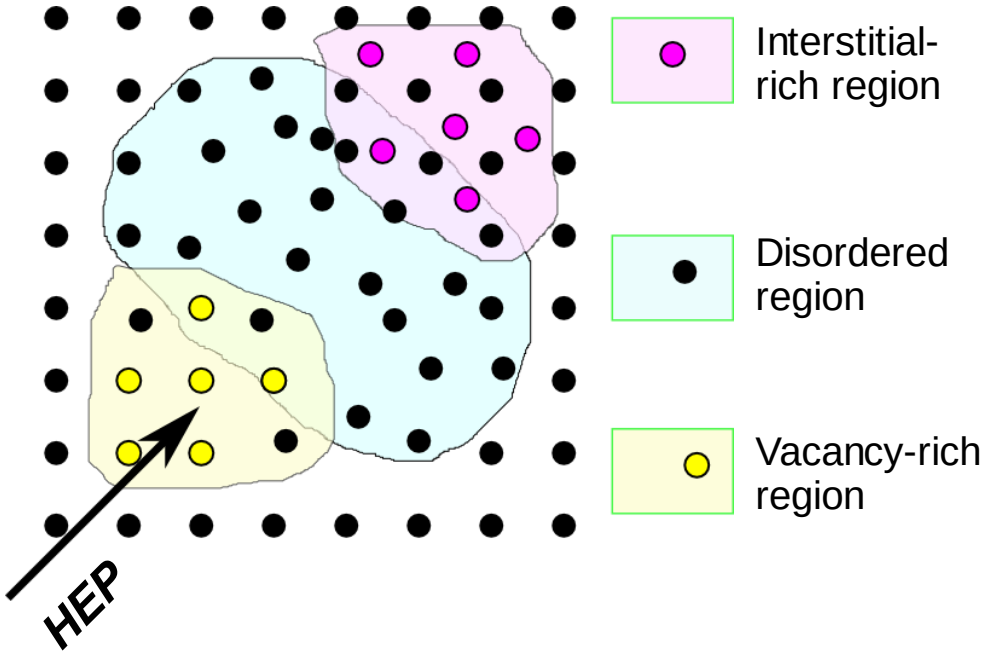
Institute of Applied Research,

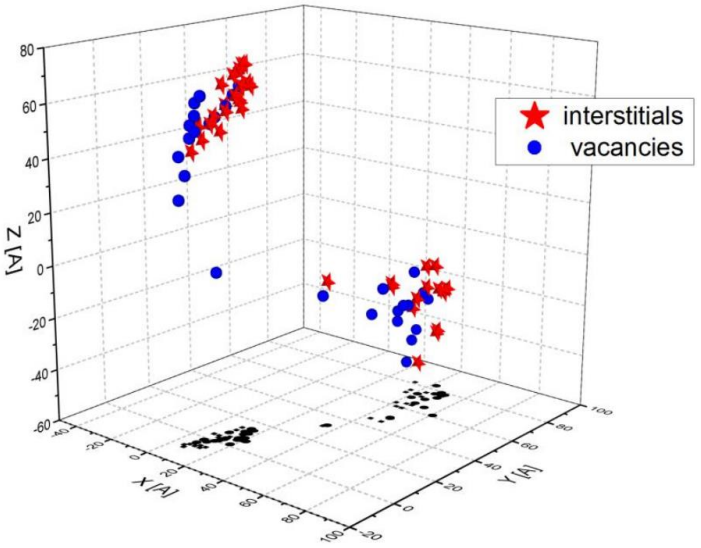
Vilnius University, Vilnius, Lithuania

Vacancy – Interstitial Defect Cluster Model Updated

Updated model:

High Energy Particle (HEP) destroys the lattice:





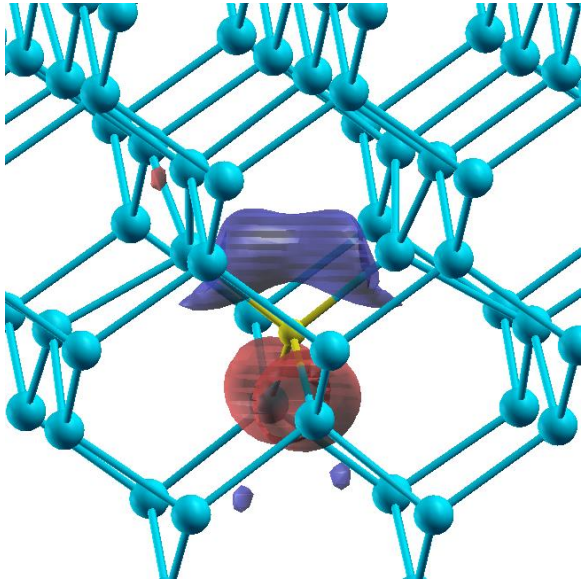
36 V/I after recombination (20%)

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

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

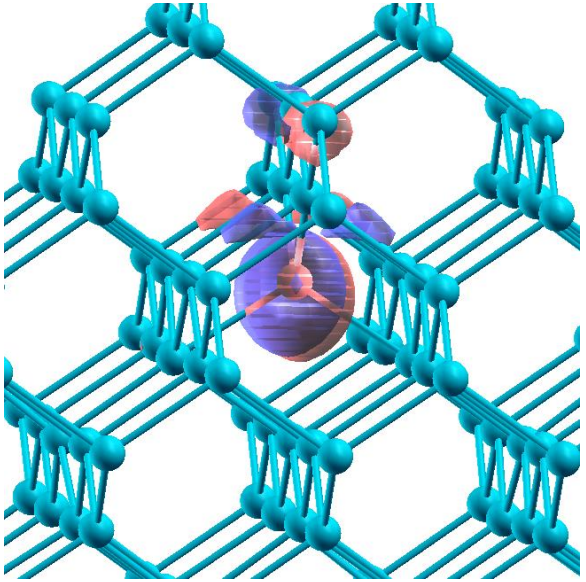
After relaxation of cascade deffect and recombination of I-V pairs the rest of the vacancies and interstitials remain separated in space.

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.

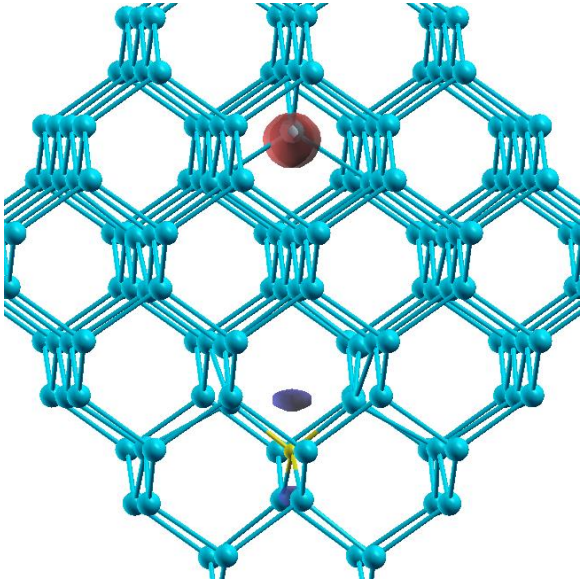
Interstitial defect in Td symmetry state is known to be of the **donor** type (Ec – 0.39 eV)
Mukashev et al, Jpn. J. Appl. Phys. 21, 399 (1982).

Here and below: Density functional calculations with ORCA program. Calculation details: the Resolution of the Identity (R-I) approximation for Coulomb energy, 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.

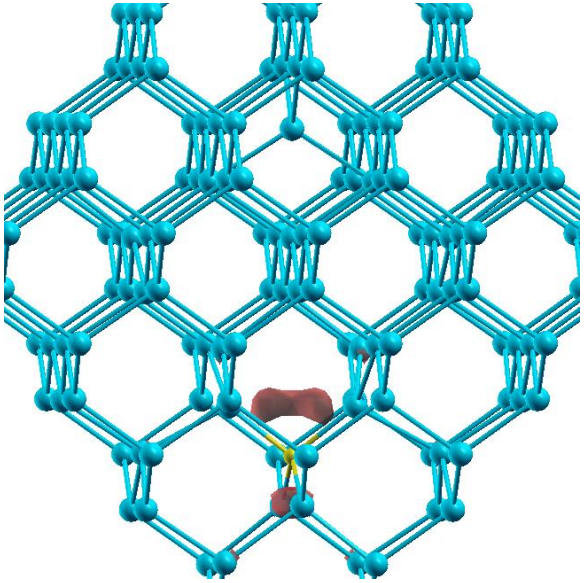
Vacancy – Interstitial pair (Frenkel pair) defect

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**:



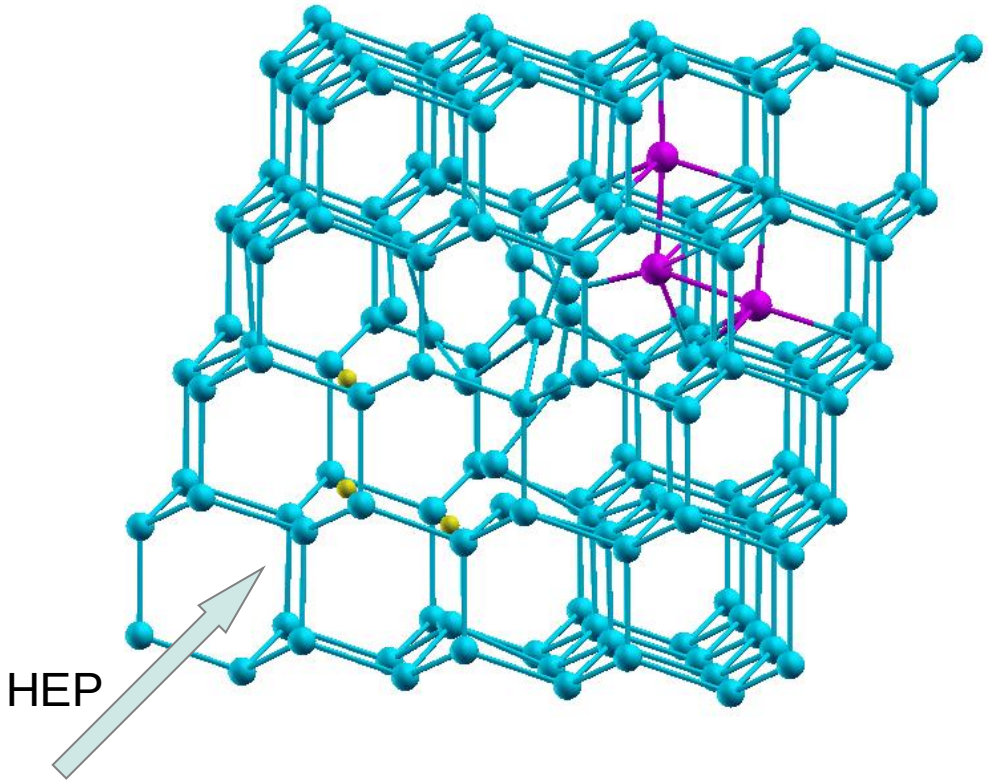
Charged (-) system, one electron added.
The **electron** wave function (~80% of it) is located nearby interstitial site (or the electron is accepted by interstitial site).



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

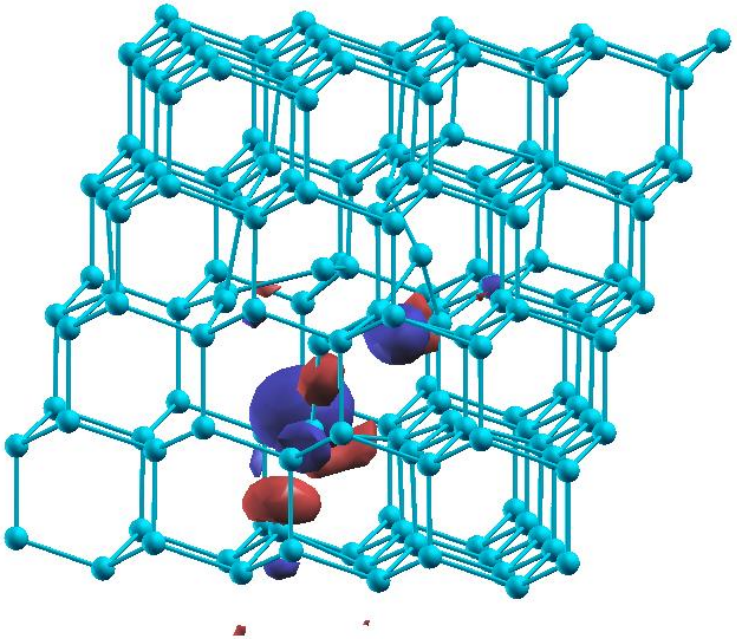


Initial structure imitating crystal structure damage by the High Energy Particle (HEP):

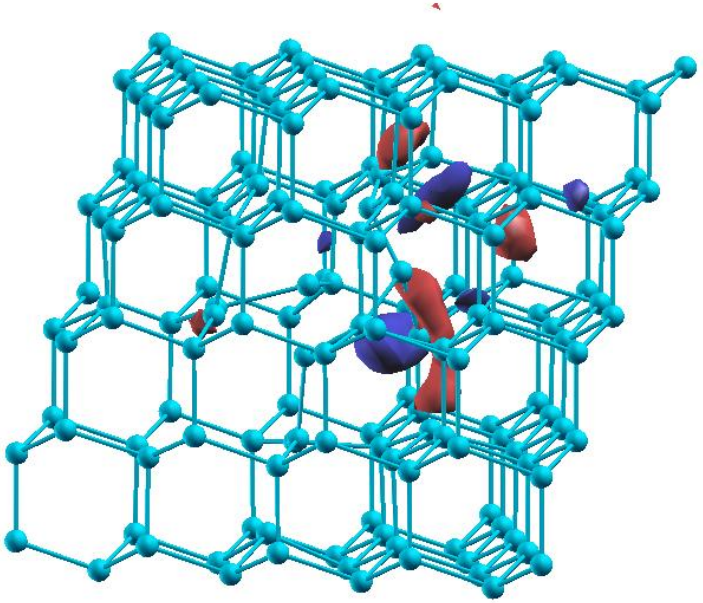
yellow are vacancy sites
magenta – interstitial Si.

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.

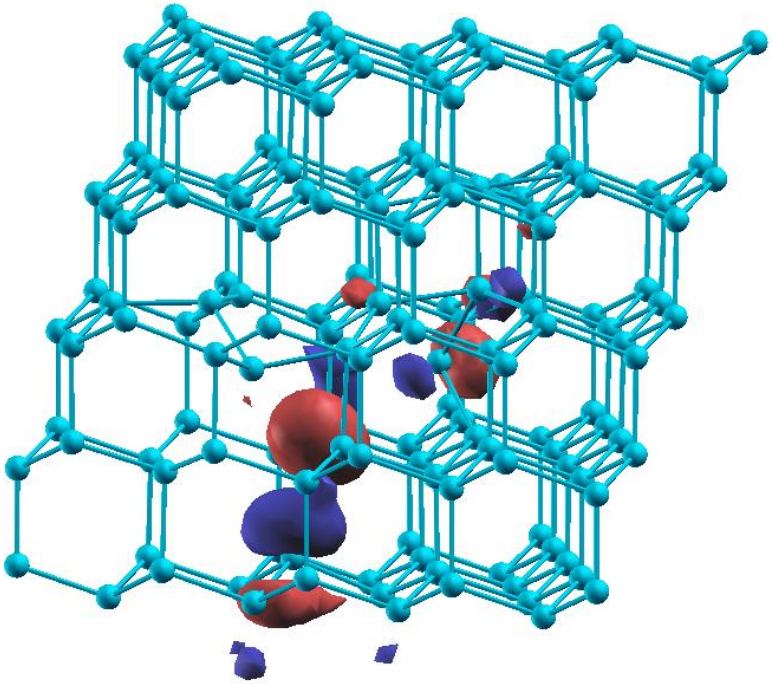


Wave function of located electron.
Electrons locate closer to interstitial-rich region.
I.e. interstitial rich region plays a role of acceptor.

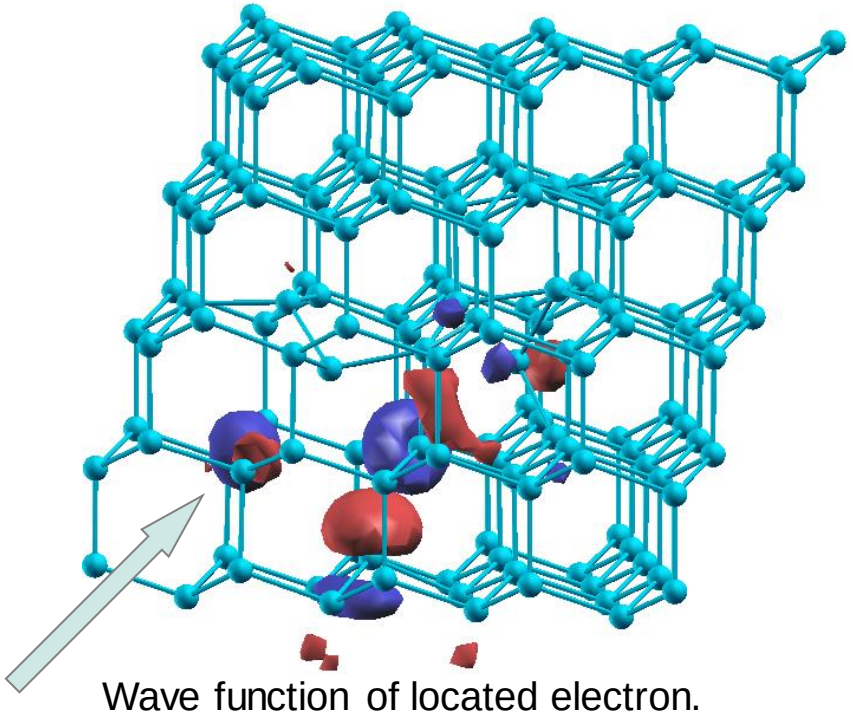
Situation is similar to the single I-V pair case.

Vacancy – Interstitial defect cluster relaxation

Fully relaxed defect structure:



Wave function of located hole.



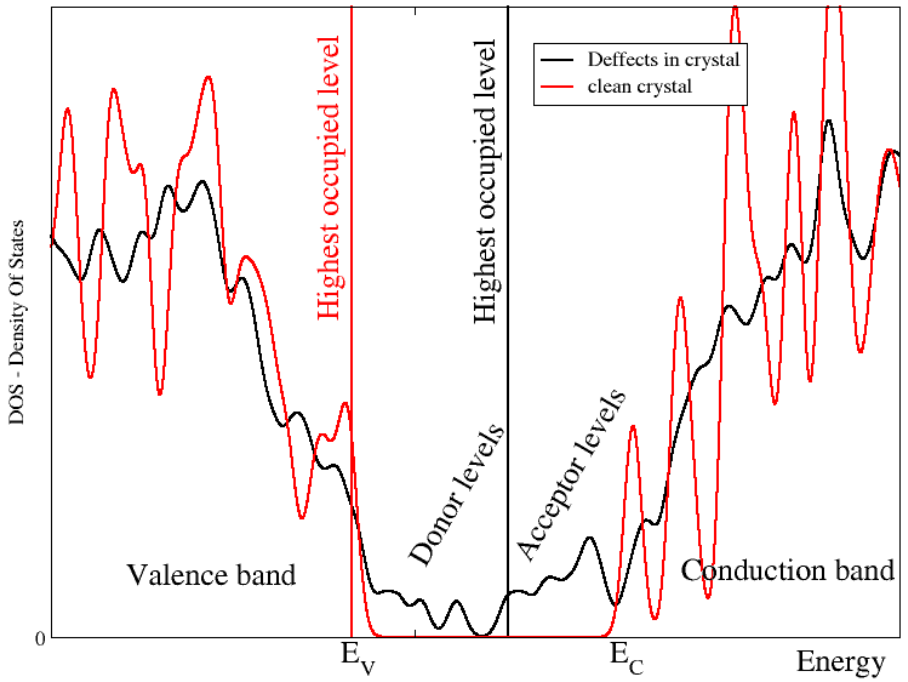
Wave function of located electron.
Part of wave function is located in vacancy region (shown by arrow).

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.

This is not a complete picture. Only one relaxation scenario was performed where interstitials where forced to relax back to the damaged region due to boundary conditions of a small cluster.
For these type of modeling one has to perform more simulation runs to get statistically important main features of cluster structure and electron states within it.
We still hope to get a defect cluster with both donor and acceptor states separated in space.

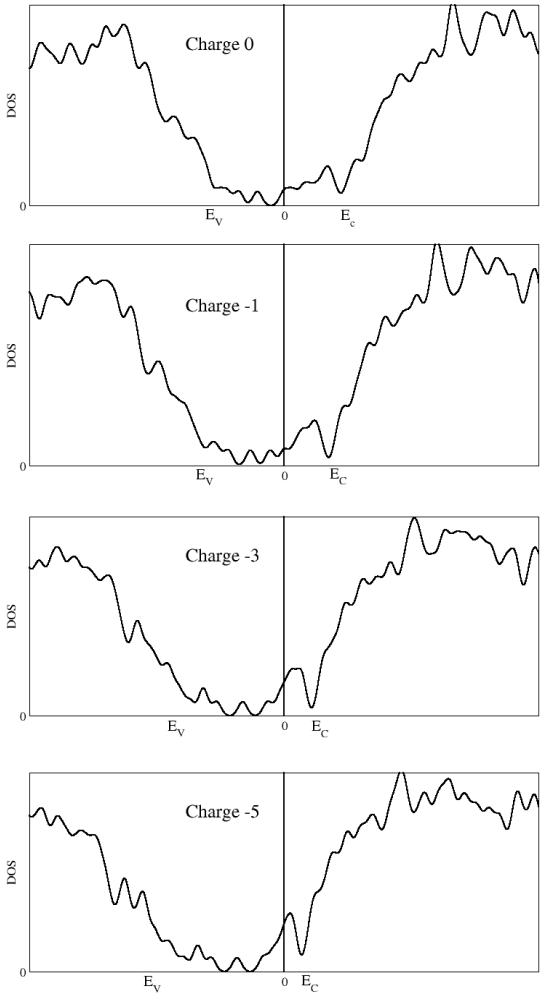
Density of states in the Vacancy – Interstitial defect cluster



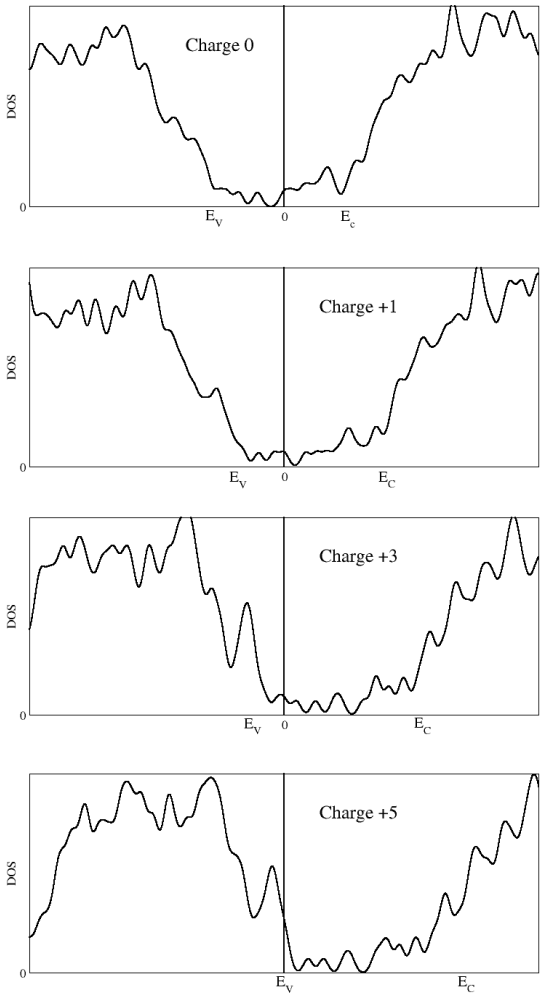
Density of states and fermi level for the defect cluster (black) compared with the same quantities of the clean Si crystal (red)

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.



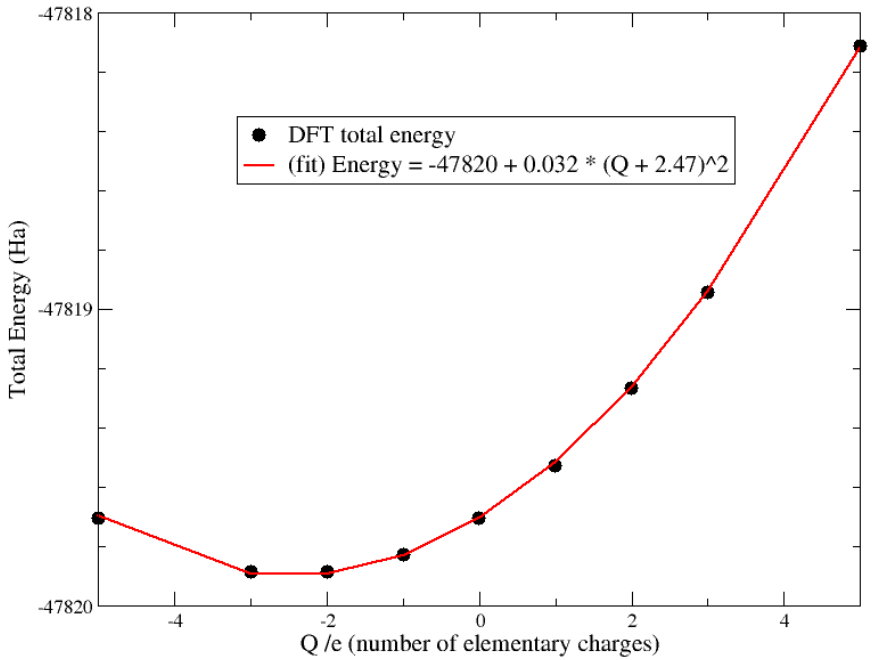
As far as we can see from the results presented here cluster may accept up to five holes and more than five (may be up to seven) electrons.
Taking 1 - 5 elementary charges per ~10 Angstrom diameter sphere one gets
~(0.2 - 1)10^{22} cm^{-3}
localized charge concentration.



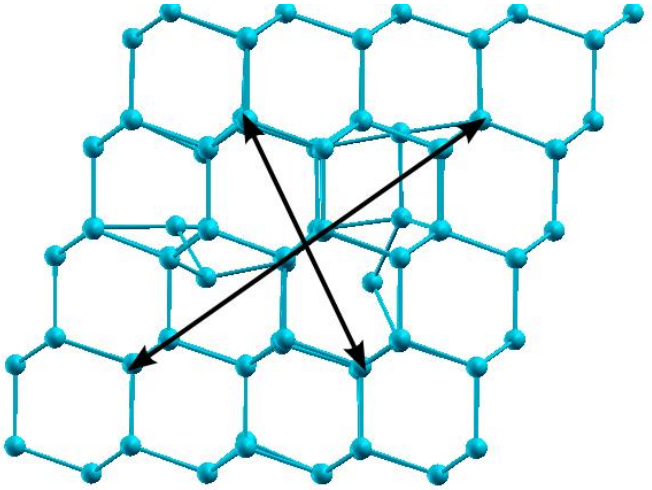
Adding electrons

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.

Mokslas • Ekonomika • Sanglauda
Europos sąjunga
Kuriame Lietuvos ateitį

This work is coherent with CERN RD50 collaboration.

Thanks to Lithuanian Science Council for the grant VP1-3.1-ŠMM-07-K-03-010

THANK YOU

FOR YOUR ATTENTION!