Multiscale Simulation of Irradiation-Induced Defect Evolution in EPI Silicon LGADs

4th DRD3 week on Solid State Detectors R&D, Nov 13, 2025

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Outline

- **Motivation**
- **Multiscale Simulation**
  - **Monte Carlo (MC) Simulation** for Primary Knock-On
  - **Molecular Dynamics (MD) Simulation** for Collision Cascade
  - **Kinetic Monte Carlo (KMC) Simulation** for Defect Evolution toward the Final State (in progress)
  - **TCAD Simulation** for Defect-Induced Electrical Performance Degradation of LGADs (in progress)
- **Summaries**

• Motivation

- **Low Gain Avalanche Detectors (LGADs)** :

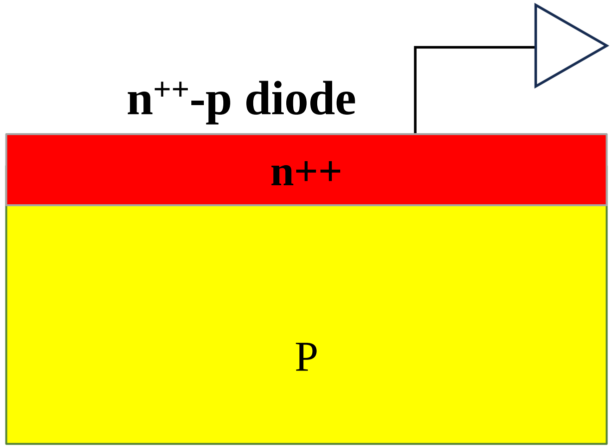
  Introducing a gain layer into the traditional PIN.

  Ultrafast time resolution.

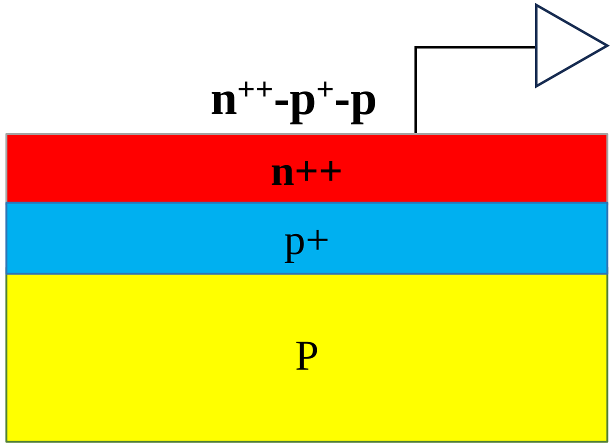
  Gain layer degradation under irradiation.

- LGADs with carbon implantation exhibit excellent radiation resistance.

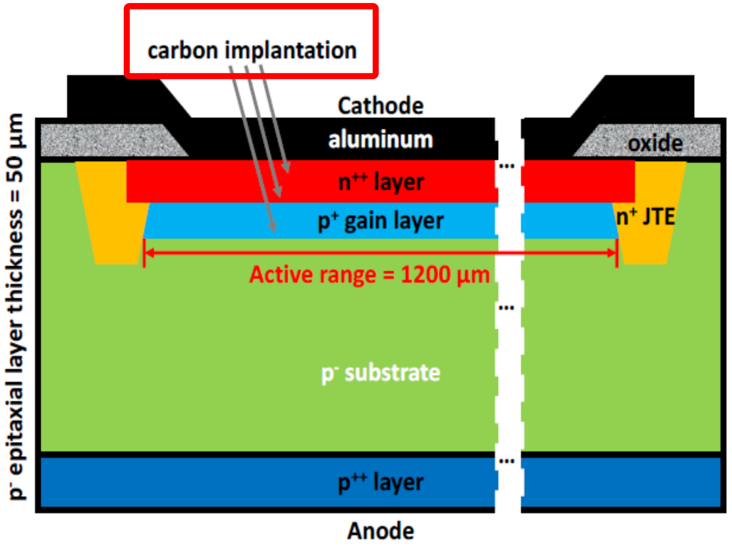
- This work aims to identify **the species and concentrations of irradiation-induced defects in LGADs**, and to evaluate **their contribution to gain degradation.**



Traditional PIN

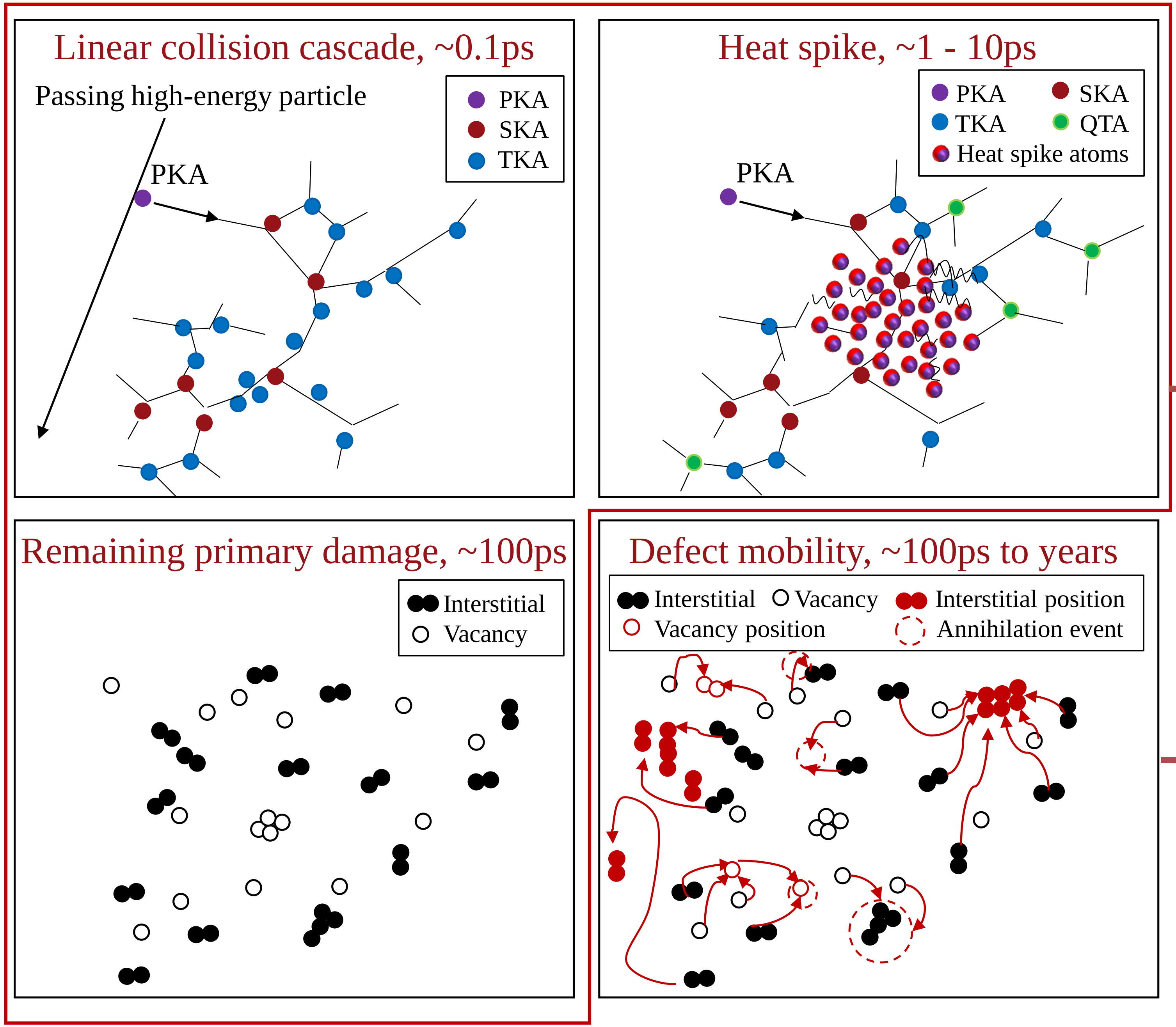


LGAD: PIN + Gain Layer



LGAD with carbon implantation

• Simulations (Method)



• Irradiation Damage Mechanism

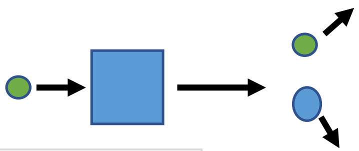
Boron typically acts as a substitutional dopant (B_s) in silicon. However, it may lose its electrical activity after irradiation.

During collision cascade (~1 to 10 ps), B_s may be directly displaced: $B_s \rightarrow B_i + V_B$?

During defect migration (~100ps to years), B_s may also be trapped by silicon Frenkel pairs: $I + B_s \rightarrow B_i$, and further combine with O_i to form more stable B_iO_i complexes: $B_i + O_i \rightarrow B_iO_i$

• Simulations (Method)

Primary displacement damage stage

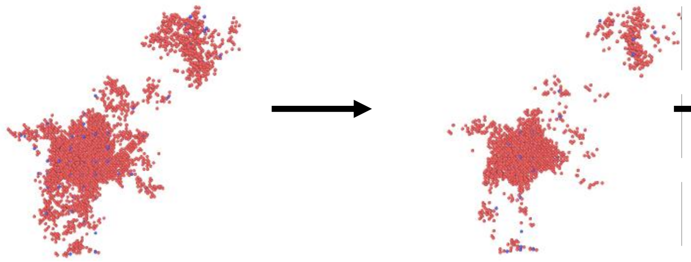


Particle incidence

PKA

MC (Geant4):
to obtain the types and energies of PKAs.

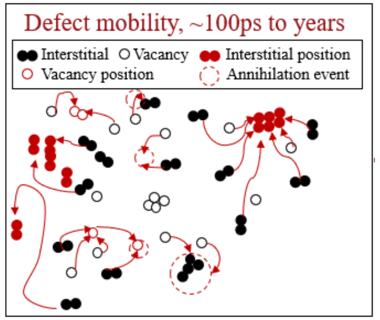
Defect evolution – short-term annealing stage



Displacement cascade

MD (LAMMPS):
to obtain the defect structure induced by displacement damage (ps, ns).

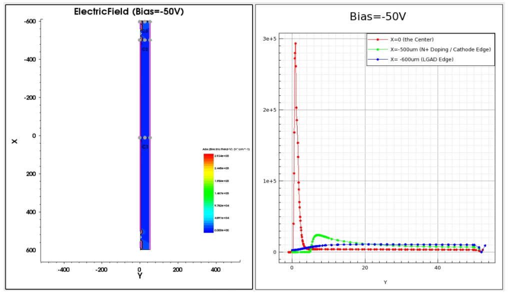
Defect evolution – long-term annealing stage



Stable defect structure

KMC (Mmonca):
to obtain the defect structure induced by displacement damage (ms, s).

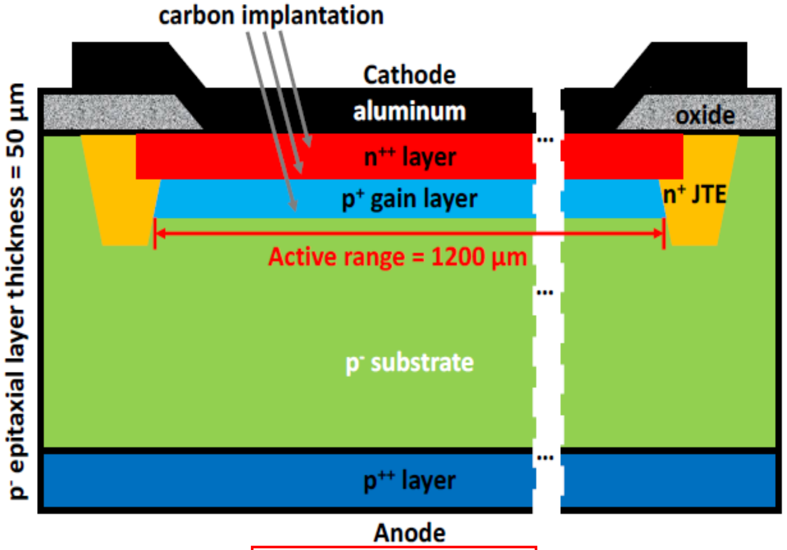
Electrical Characteristics



TCAD:
to obtain the impact of defects on the macroscopic electrical characteristics of LGADs

• Simulations (MC)

• Modelling in Geant4

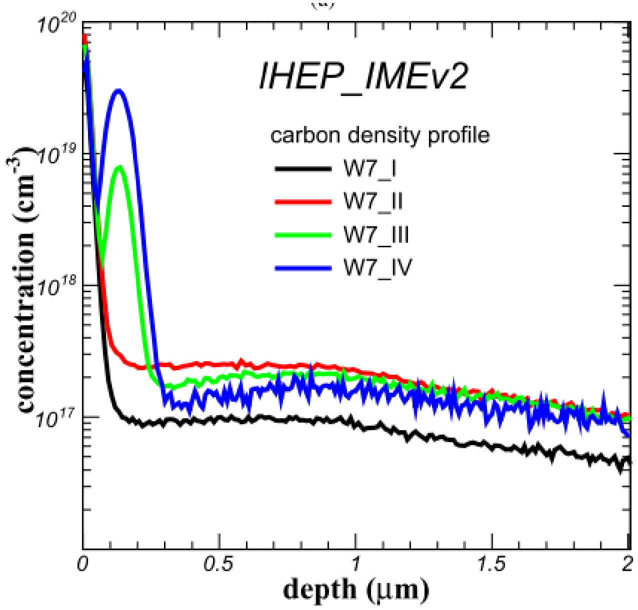


1MeV neutron

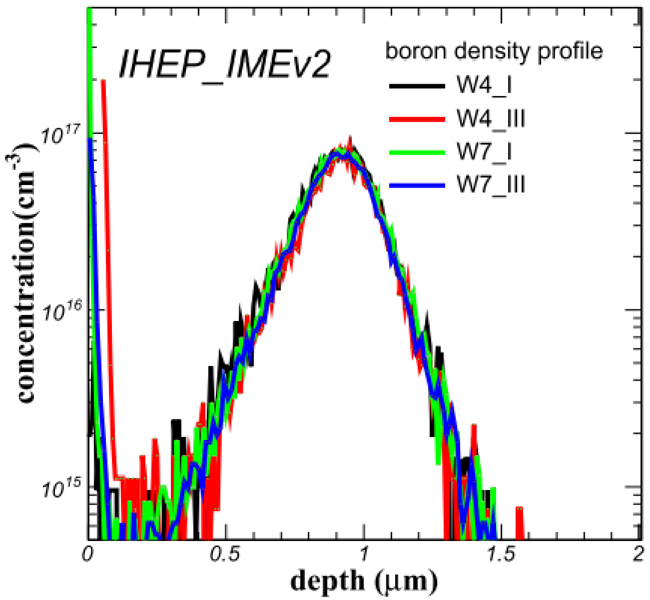
Al, 0.3μm
0-0.5μm, Si+C(2E17)
0.5-0.75μm, Si+B(5E15)+C(2E17)
0.75-1.25μm, Si+B(5E16)+C(2E17)
1.25-1.5μm, Si+B(5E15)+C(2E17)
1.5-2μm, Si+C(2E17)
Si_Base, 48μm

- **What do we want from the G4 simulation?**

The energy distribution and spatial distribution of PKAs.



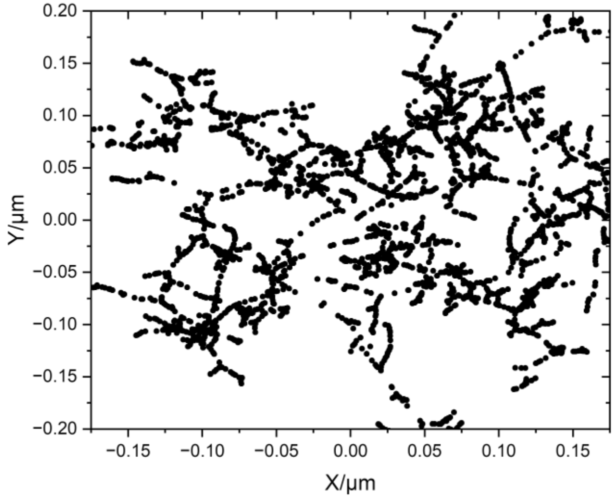
Carbon Density Profile by SIMS[5]

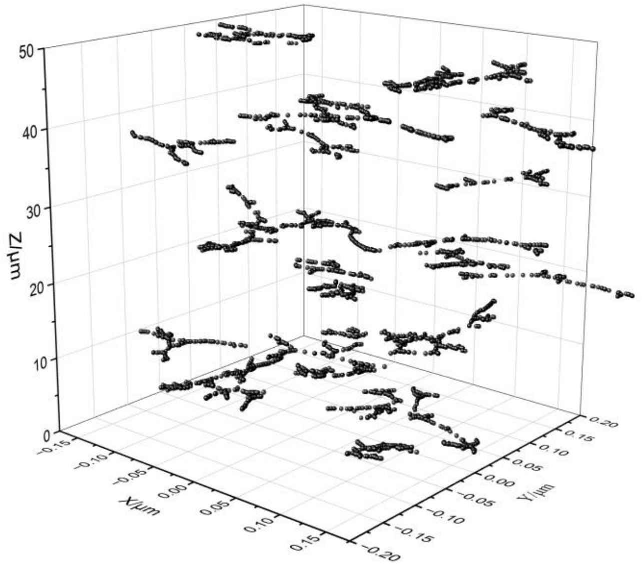


Boron Density Profile by SIMS [5]

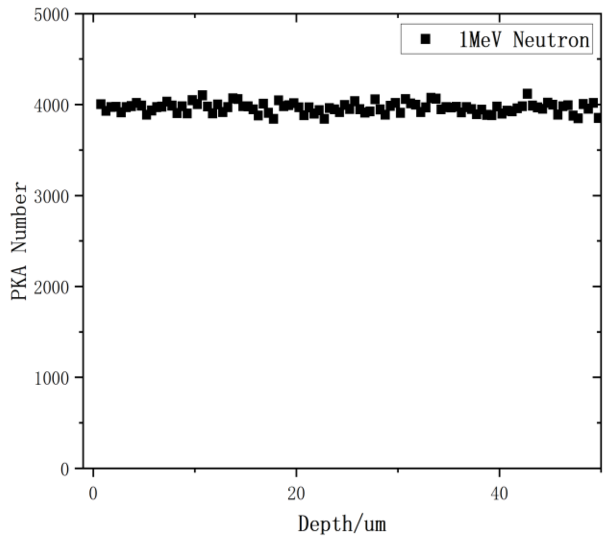
- **Physics List:** QGSP_BIC; G4ScreenedNuclearRecoil
- **Theoretical Model:** Lindhard Funtion; Norgett-Robinson-Torrens (NRT) Model
- **Particle Source**: Face Source (1MeV Neutron); Perpendicular Incidence;

• Simulations (MC)

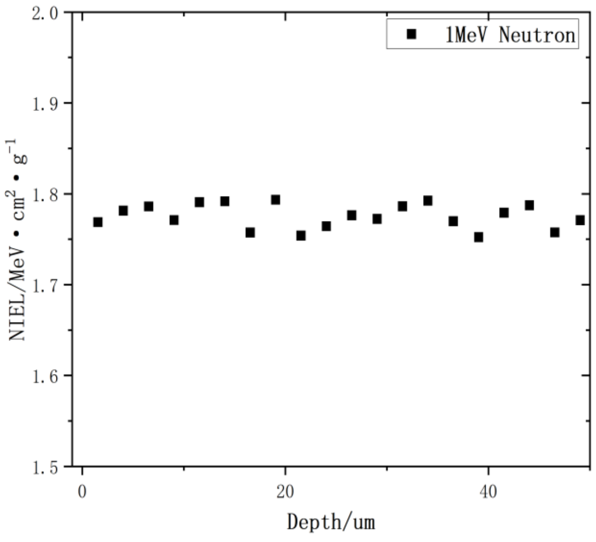




Distribution of vacancies by Geant4 (1MeV Neutron)



Depth distribution of PKA number (1MeV Neutron)



Depth distribution of NIEL (1MeV Neutron)

- **To calculate Parameter L in MC**： L is the number of vacancies generated per unit length by each incident neutron.

Radiation-induced vacancy defects are **uniformly distributed** along the X, Y and Z directions. Thus, the results of local defects can represent the whole.

The uniform distribution of vacancies is due to the fact that the NIEL deposited and the number of PKAs generated by neutrons are consistent along the Z direction.

• Simulations (MC)

- **To calculate Parameter L**： L is the number of vacancies generated per unit length by each incident neutron.

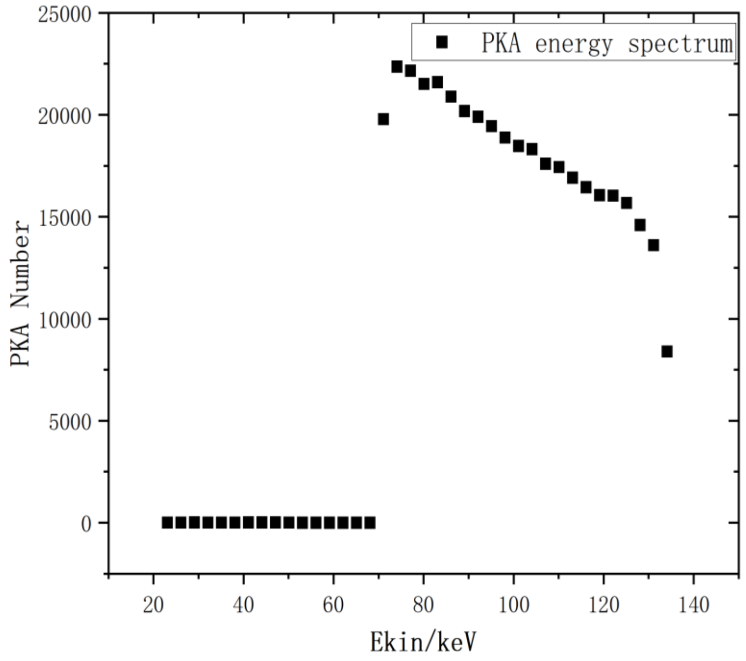
NRT Model:

$$N_d(T) = \begin{cases} 0 & T > E_d \\ 1 & E_d \le T \le 2.5E_d \\ \frac{0.8(T)}{2E_d} & T \ge 2.5E_d \end{cases}$$

$$L = \frac{\text{Average Nd per neutron}}{h}$$

Average Nd per neutron	L in SIMS /cm^{-1}	L in Simulation /cm^{-1}
0.295234899	52.5	59.047

- **To obtain information about PKAs**, which is taken as the input for MD simulations.

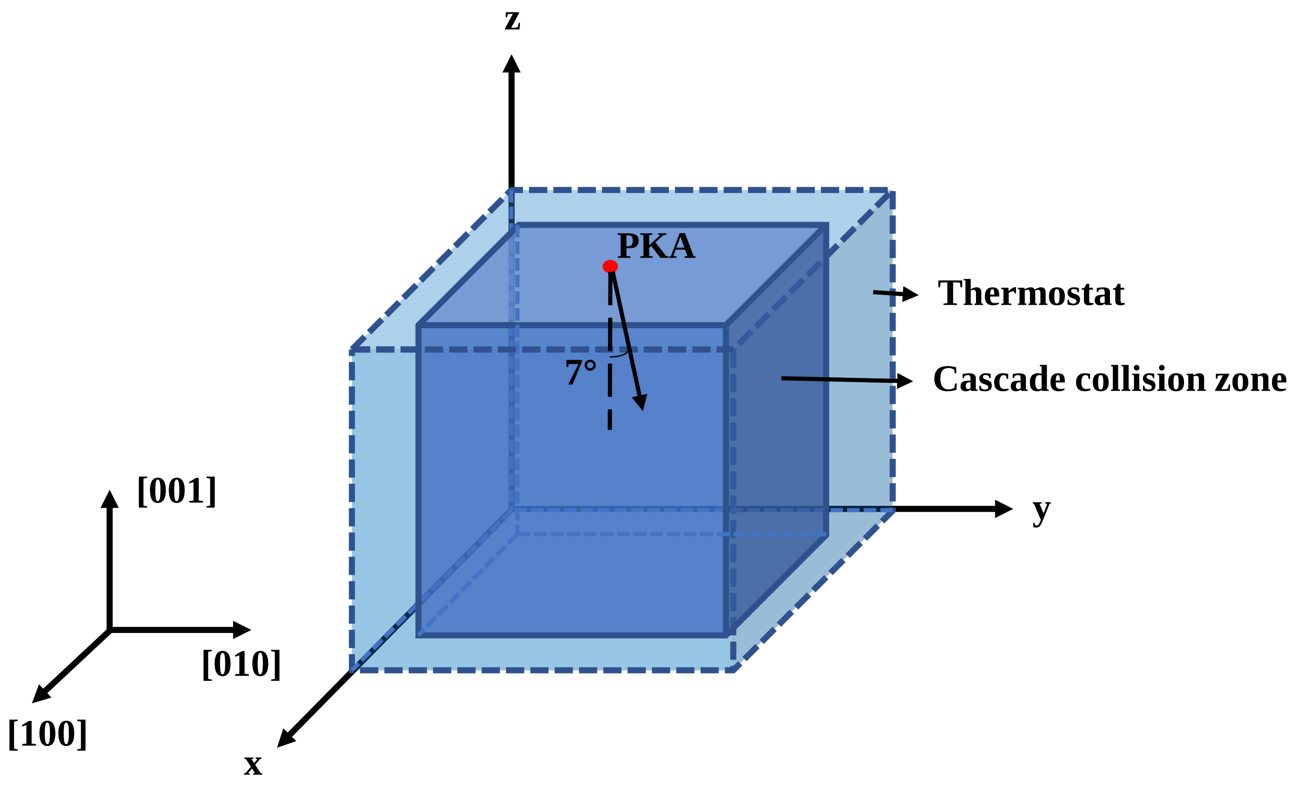


PKA Energy Spectrum (1MeV Neutron)

The PKA energy ranges from 70 to 133 keV, with 72.6 keV being the most probable value.

• Simulations (MD)

• Modelling in LAMMPS



MD Modeling of Cascade Collision Systems in Silicon (50×50×50, i.e., 271.99×271.99×271.99 Å^3)

• Three Systems

1. Bs-doping in Si

Potential: Stillinger-Weber (SW))[8]

2. Cs-doping in Si

Potential: Tersoff/ZBL

3. Oi-doping in Si

Potential: Tersoff/ZBL

During the cascade collision process, is the interaction of Bs being directly knocked out (Bs → Bi + VB) worth considering?

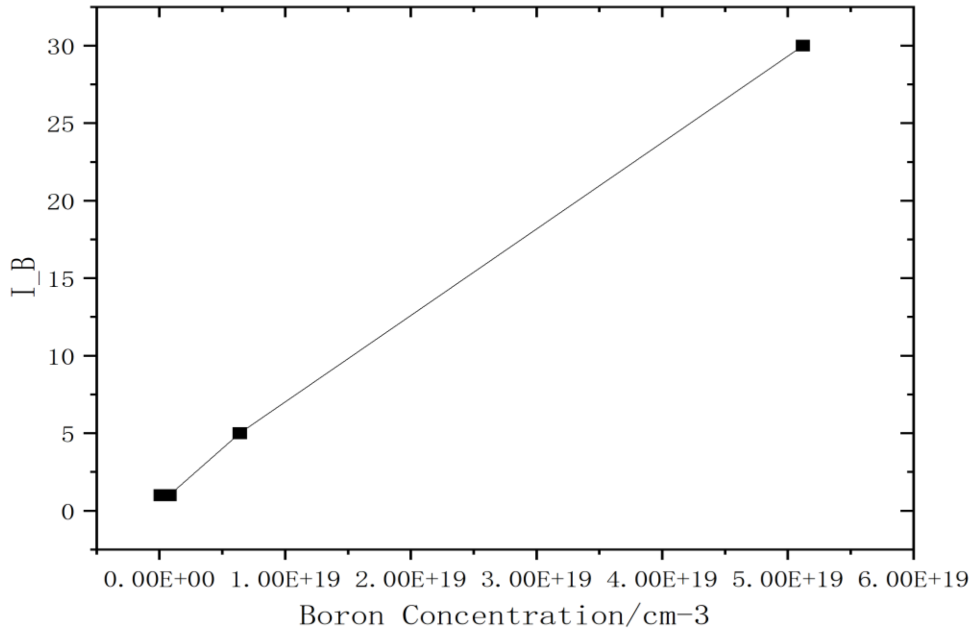
• Simulations (MD)

• Modelling in LAMMPS

	B_s	C_s	O_i	Assumption for Increasing the Doping Concentration					
Actual Doping Concentration/cm^{-3}	1.00E+17	2.00E+17	2.00E+17	1E17	4.1E17	8E17	6.4E18	5.12E19	8E20
One Dopant Atom per A*B*C Lattice Sites	40*40*40	31*31*31	31*31*31	40*40*40	25*25*25	20*20*20	10*10*10	5*5*5	2*2*2

- Due to the low actual doping concentration, it is challenging to directly capture its effect in MD simulations.

- To demonstrate that the doping concentration can be reasonably extrapolated, allowing high-concentration results to represent low-concentration.



The relationship between the number of B_i and boron concentration

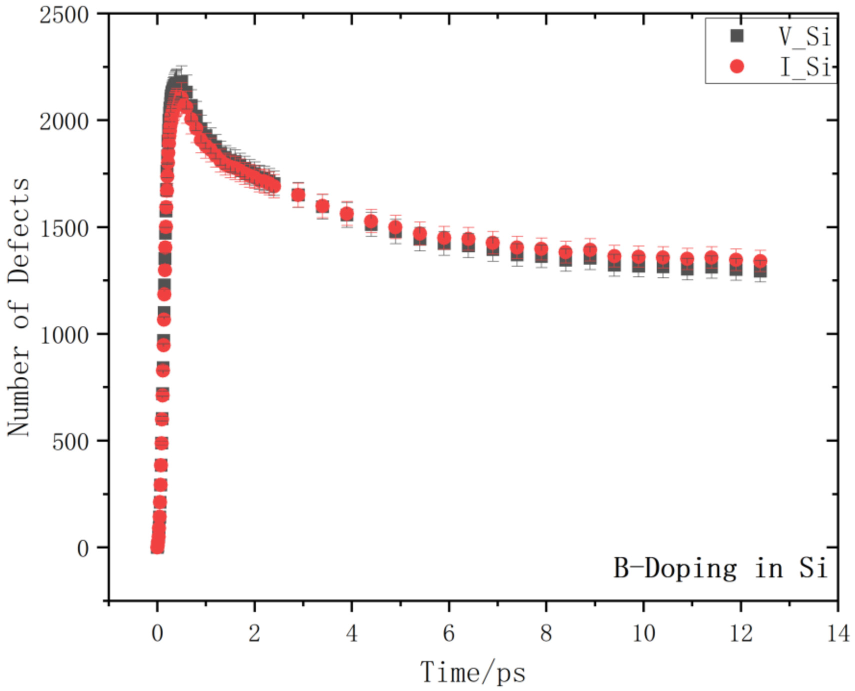
• Simulations (MD)

Actual B concentration / cm^{-3} →

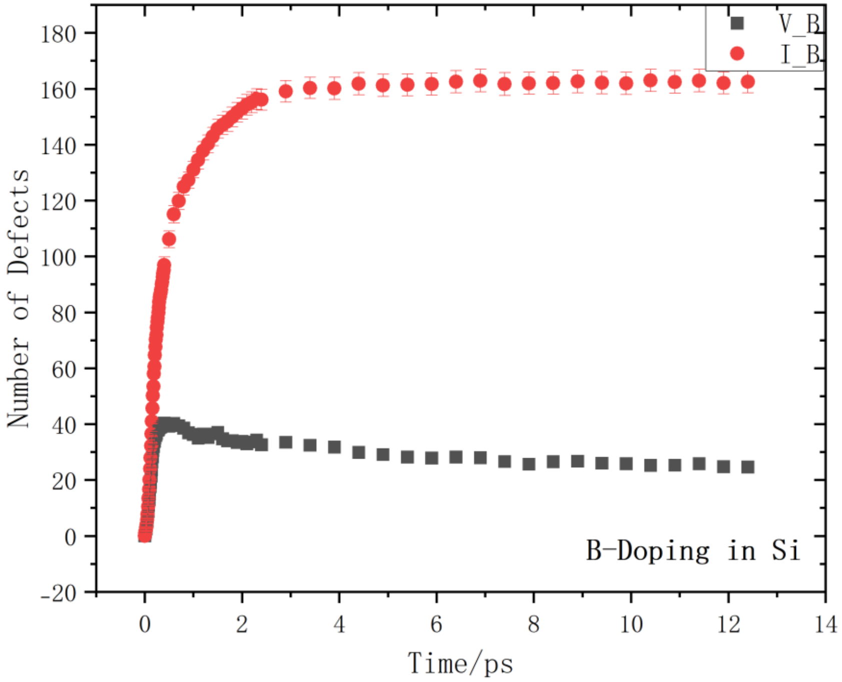
B_s
1.00E+17
40*40*40

B concentration used in this simulation/ cm^{-3} →

5.12E19
5*5*5



Evolution of the Number of Defects Over Time: V_{Si}, I_{Si}

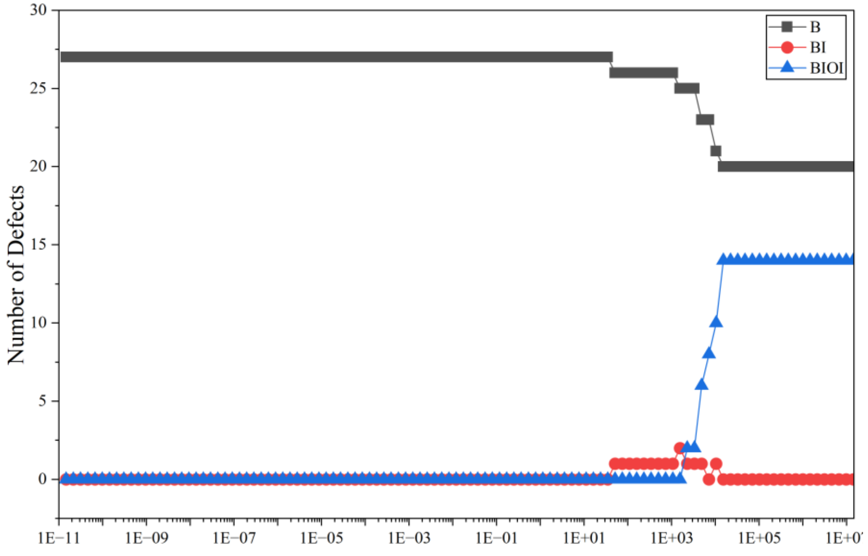


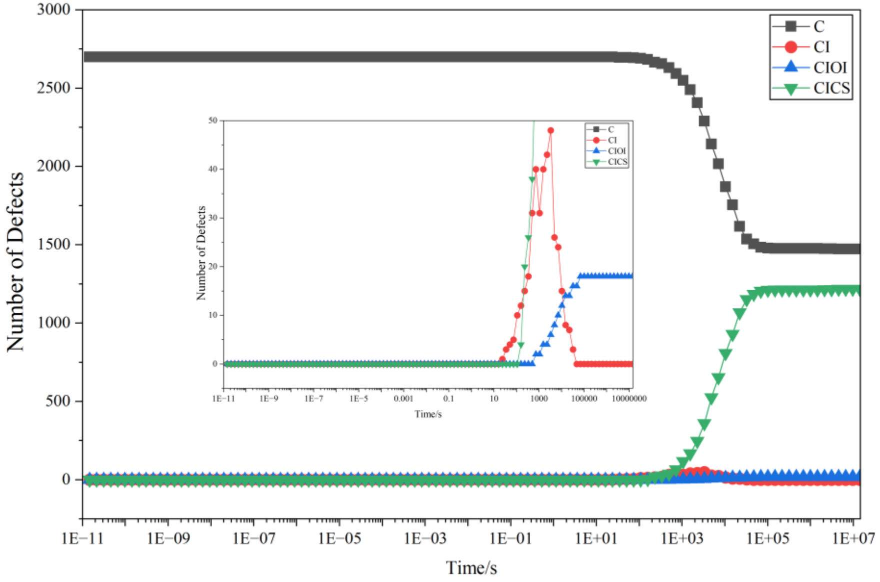
Evolution of the Number of Defects Over Time: V_B, B_i

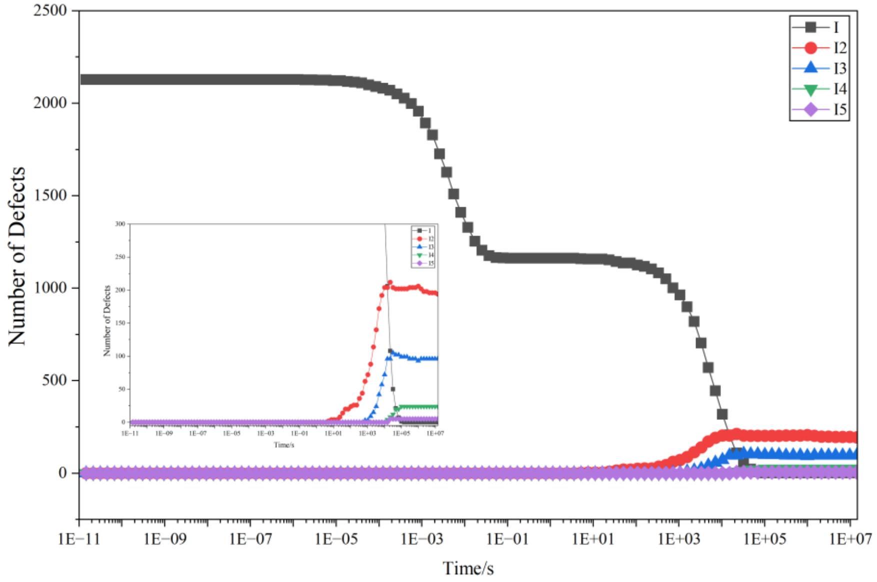
- A single PKA in the system can only produce 0.317 ± 0.008 Bi defects on average, which is very low compared to Si-Frenkel pairs.
- Thus: during the cascade collision process, the probability of Bs being directly knocked out (Bs → Bi + VB) is extremely low and negligible.
- Our ultimate focus is on the long-term evolution of defects after the cascade collision ends (e.g., I + Bs → Bi, Bi + Oi → BiOi).

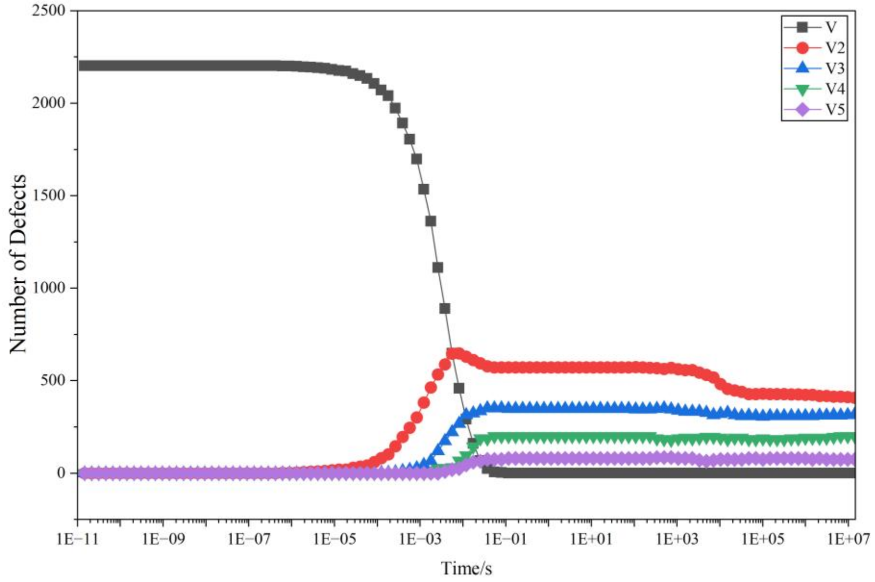
• Simulations (KMC)

B： 1E17 cm^{-3}； C： 1E19 cm^{-3}； O： 2E17 cm^{-3}





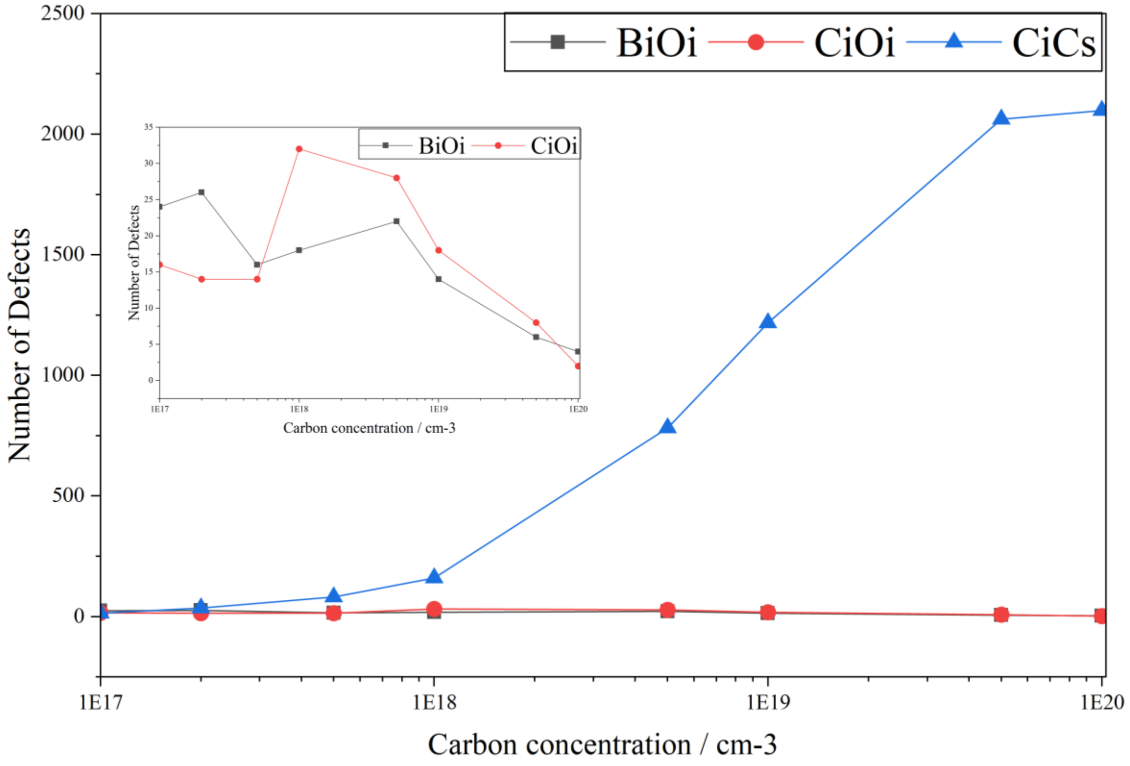




- KMC simulation aims to determine the steady-state configuration of defects upon long-term evolution.
- Thus far, this study has quantified the final concentrations of various defects, including B_s, C_s, B_i, C_i, BiOi, CiOi, CiCs, I/I clusters, and V/V clusters.

• Simulations (KMC)

The impact of different carbon doping concentrations on the formation of B-related and C-related defects.



- BiOi and CiOi: We observed that the concentrations of both BiOi and CiOi defects generally decrease as the carbon doping concentration increases.

- CiCs: We found that as the carbon concentration increases, the dominant form of C-related defects becomes CiCs, and the concentration of this defect tends to saturate when the carbon doping level reaches 1×10^{20} cm^{-3}. This may represent the microscopic mechanism by which carbon doping enhances the radiation tolerance of LGADs.

Summaries

- **We aim to developed a multi-scale simulation framework (MC→MD→KMC→TCAD) to study irradiation-induced defect types and distributions in LGADs**, ultimately aiming to identify defects most critical to gain degradation. Current results provide concentrations for BiOi , CiOi, CiCs, I/V and their clusters. Subsequent work will focus on the impact of these defects on the electric field distribution.
- We found that as the carbon concentration increases, the dominant form of C-related defects becomes CiCs, and the concentration of this defect tends to saturate when the carbon doping level reaches 1×10^{20} cm^{-3}. This may represent the microscopic mechanism by which carbon doping enhances the radiation tolerance of LGADs.

Thanks for your attention!

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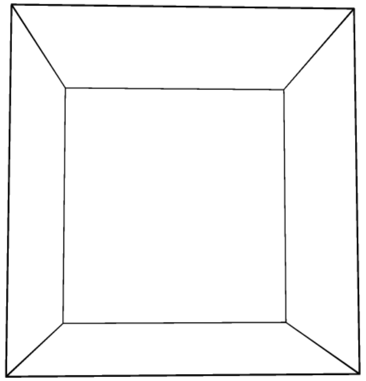
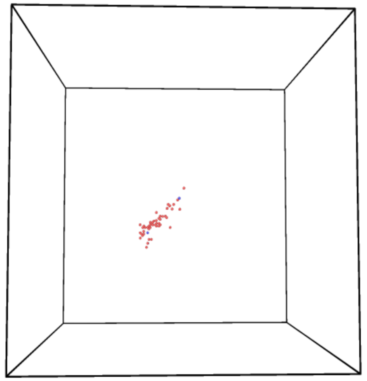
MD simulation: B-Doping in Si (Interatomic Potential : Stillinger-Weber (SW) [8])

Spatial Distribution of All Vacancies and Interstitial Defects


0ps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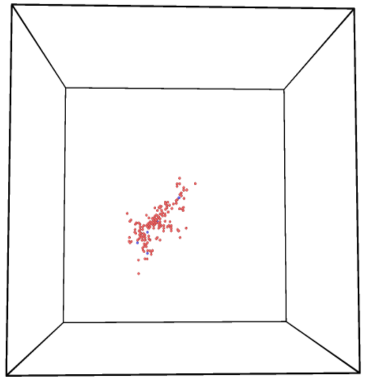
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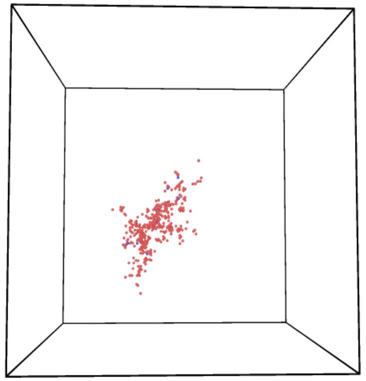
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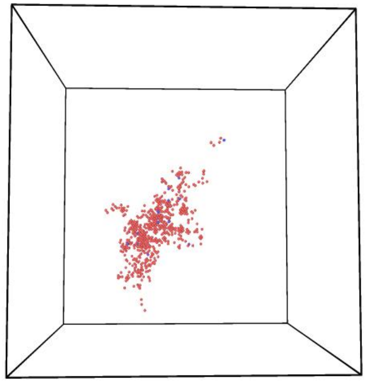
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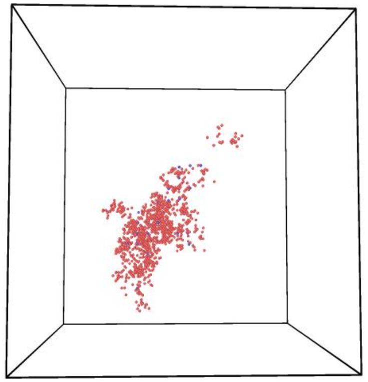
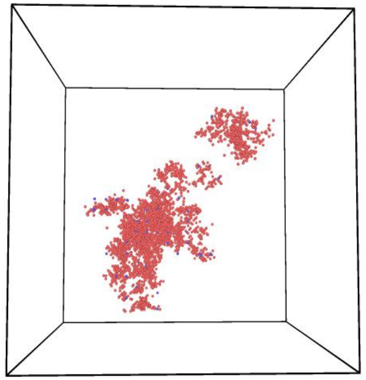

0.1ps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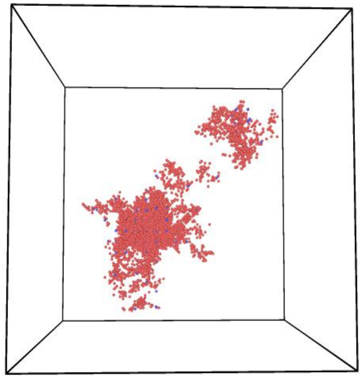
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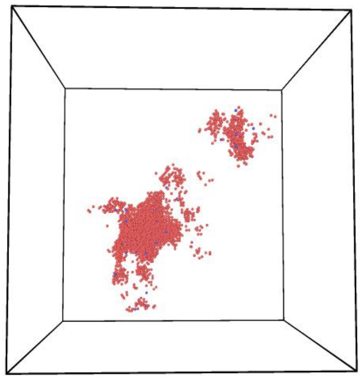
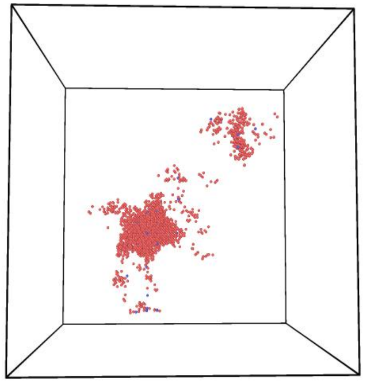
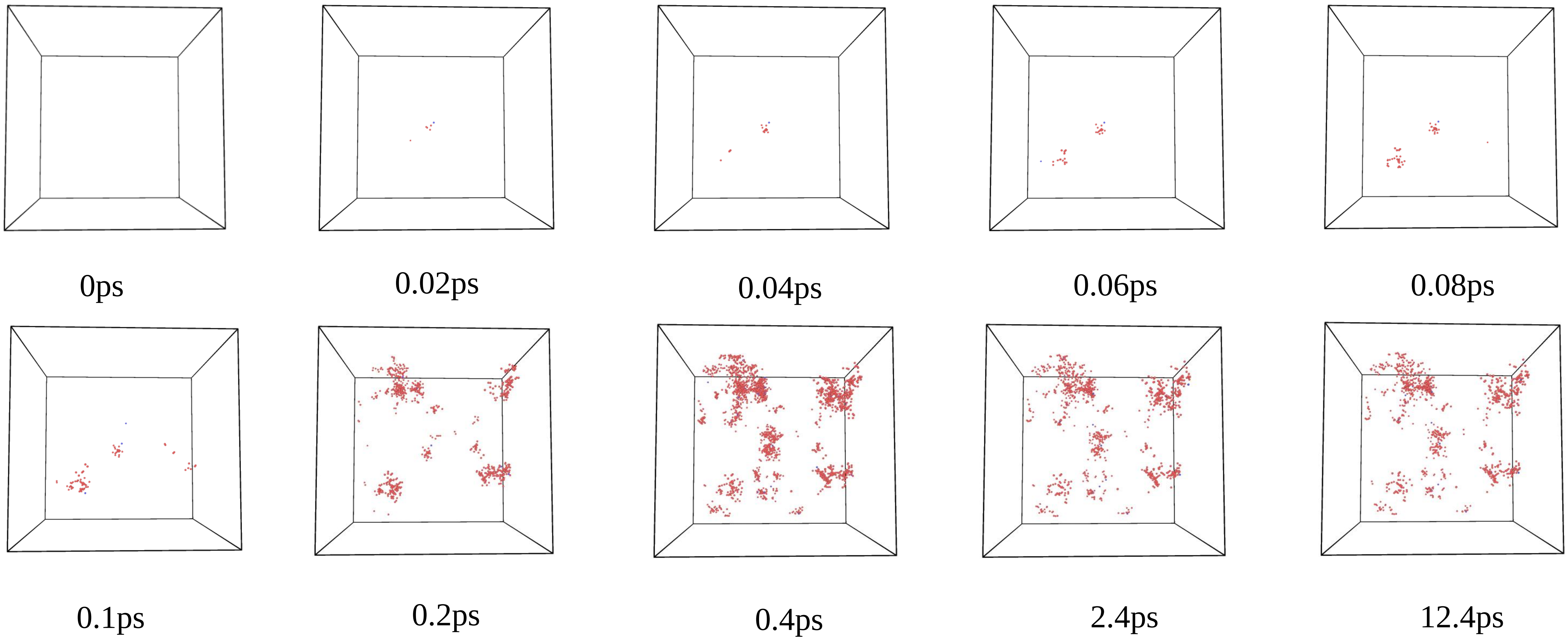

2.4ps


12.4ps

MD simulation: C-Doping in Si (Interatomic Potential : Tersoff/ZBL)

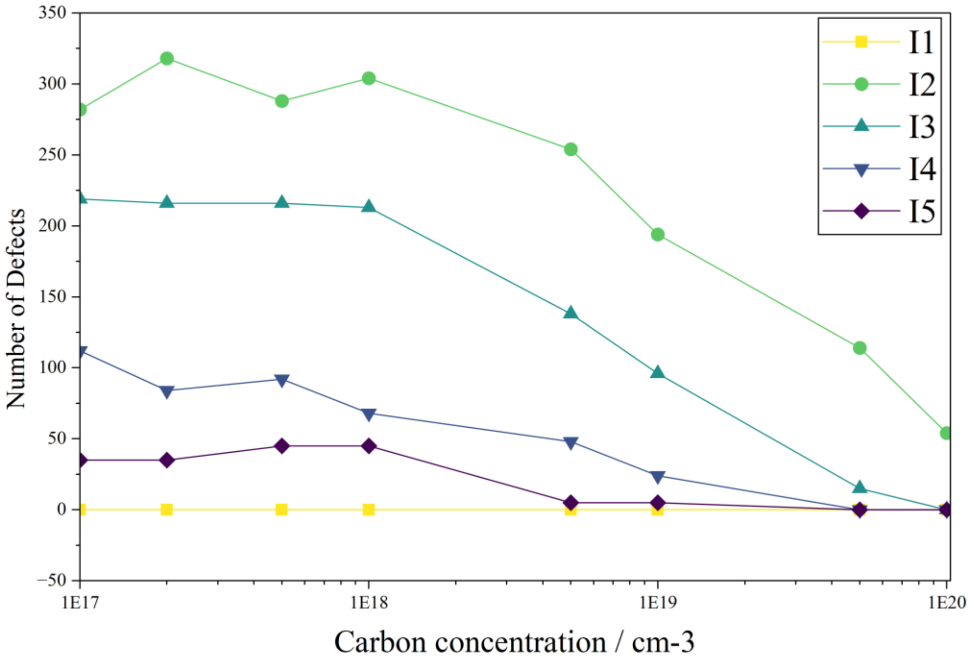
Spatial Distribution of All Vacancies and Interstitial Defects

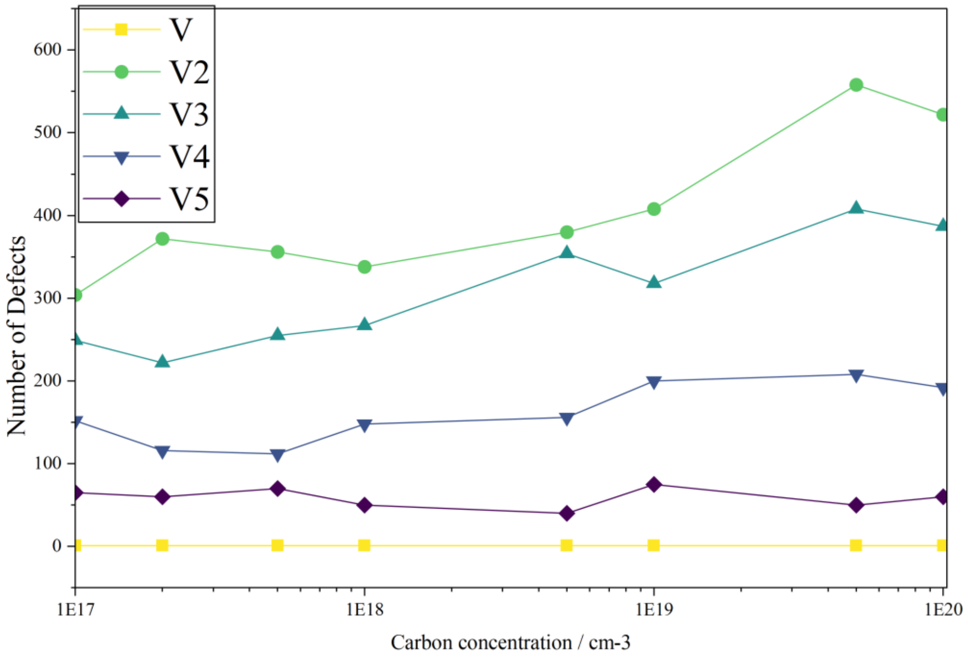


• Backup

- Simulations (KMC)

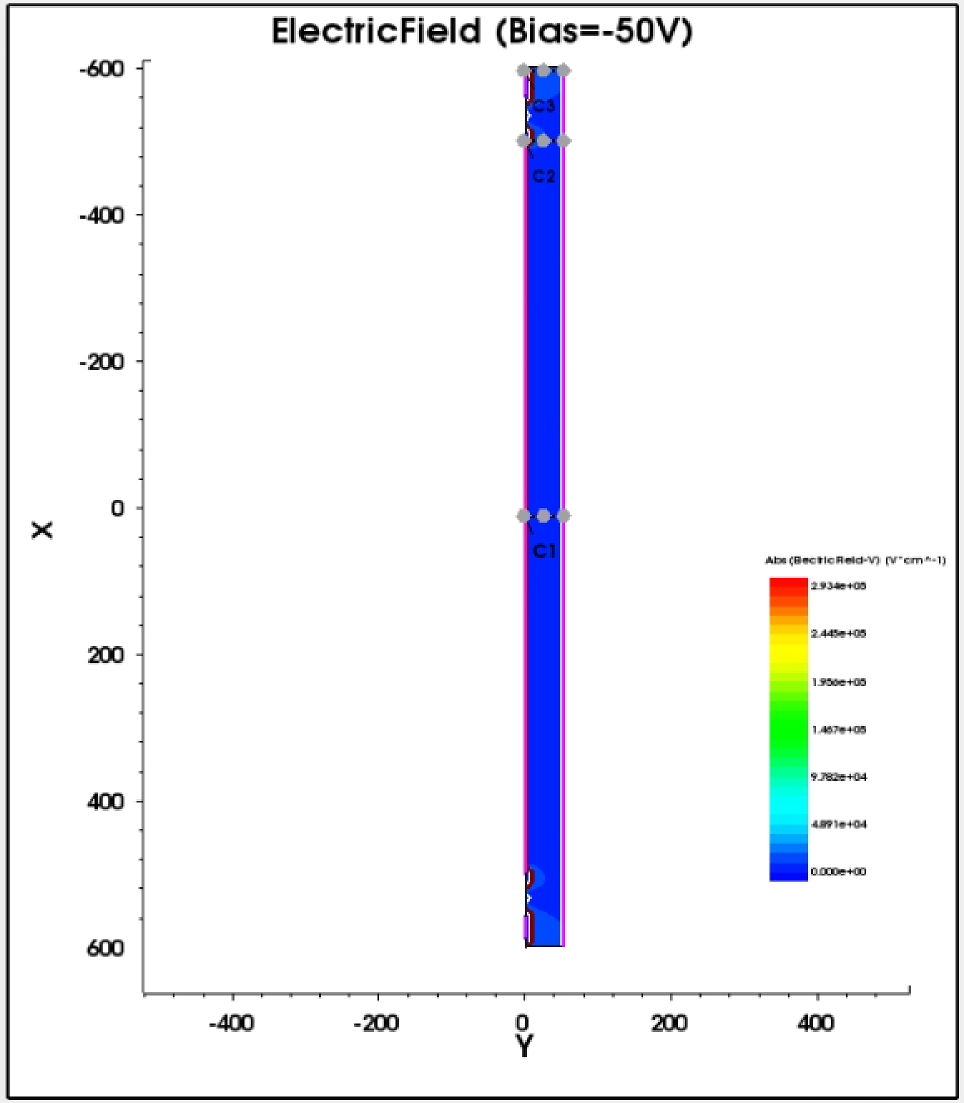
The impact of different carbon doping concentrations on the formation of I-related and V-related defects.

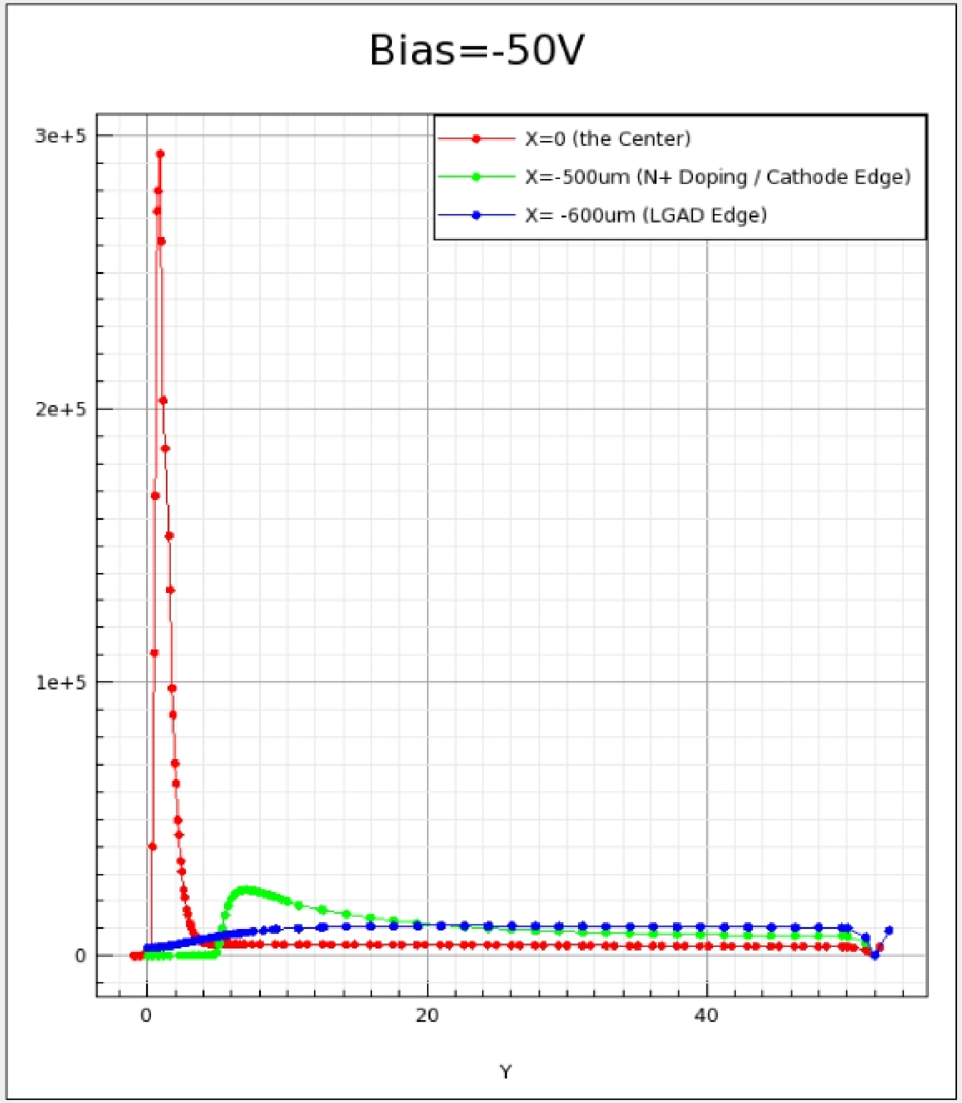




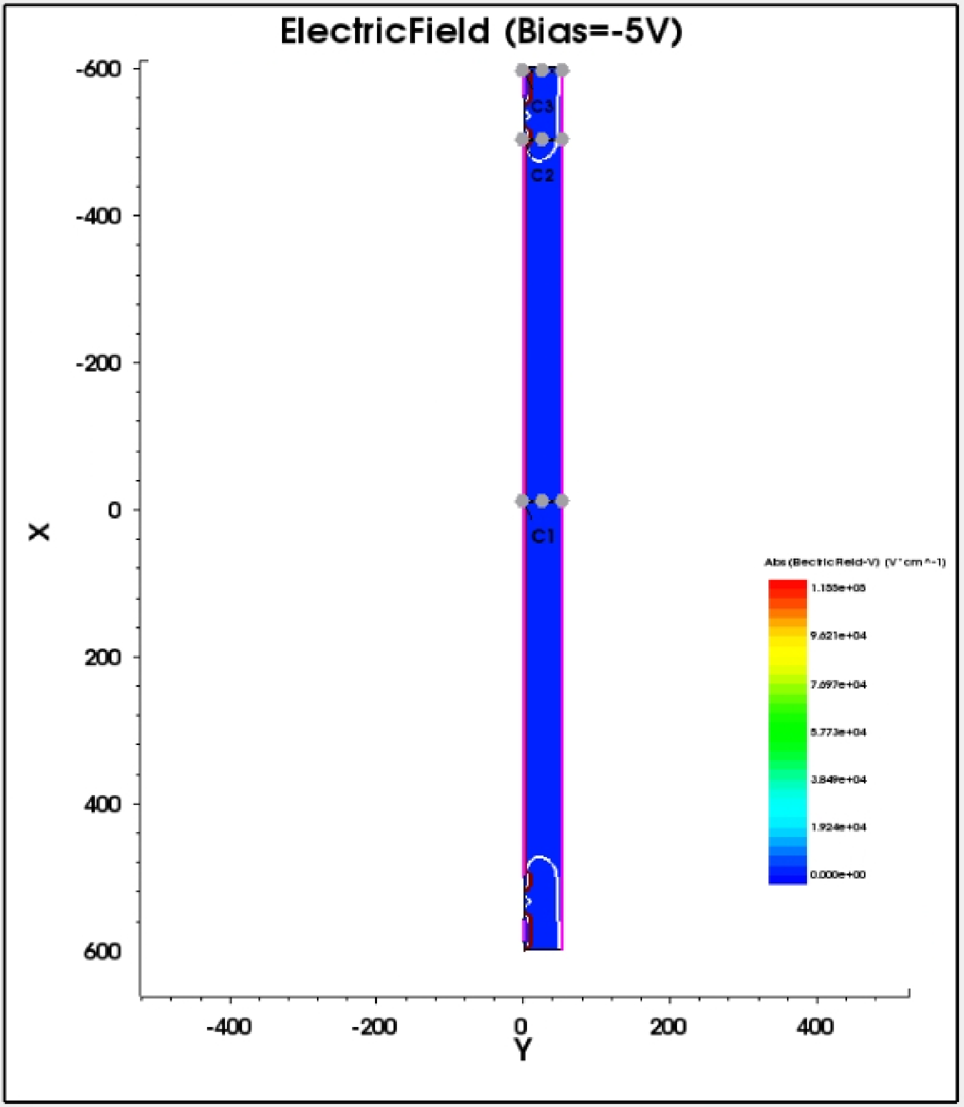
• Backup

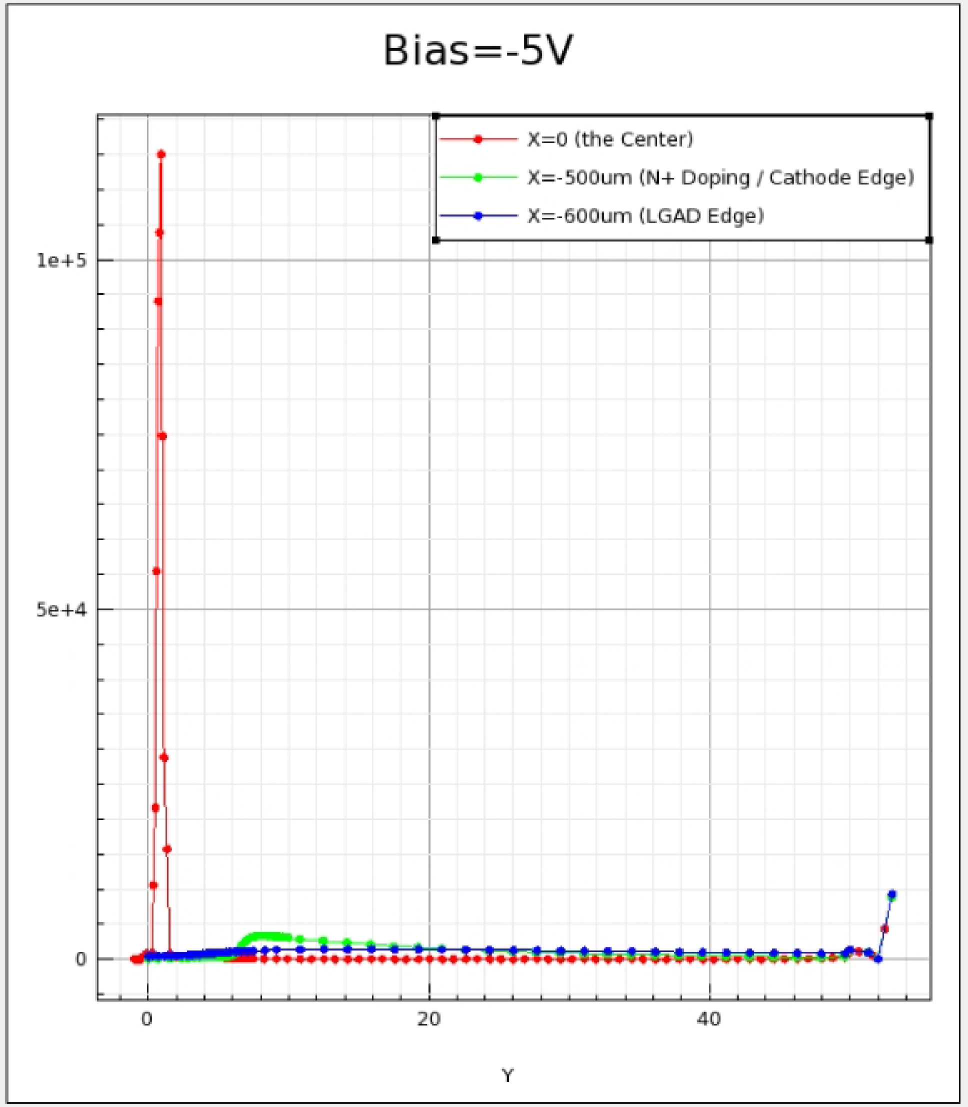
TCAD: ElectricField-V





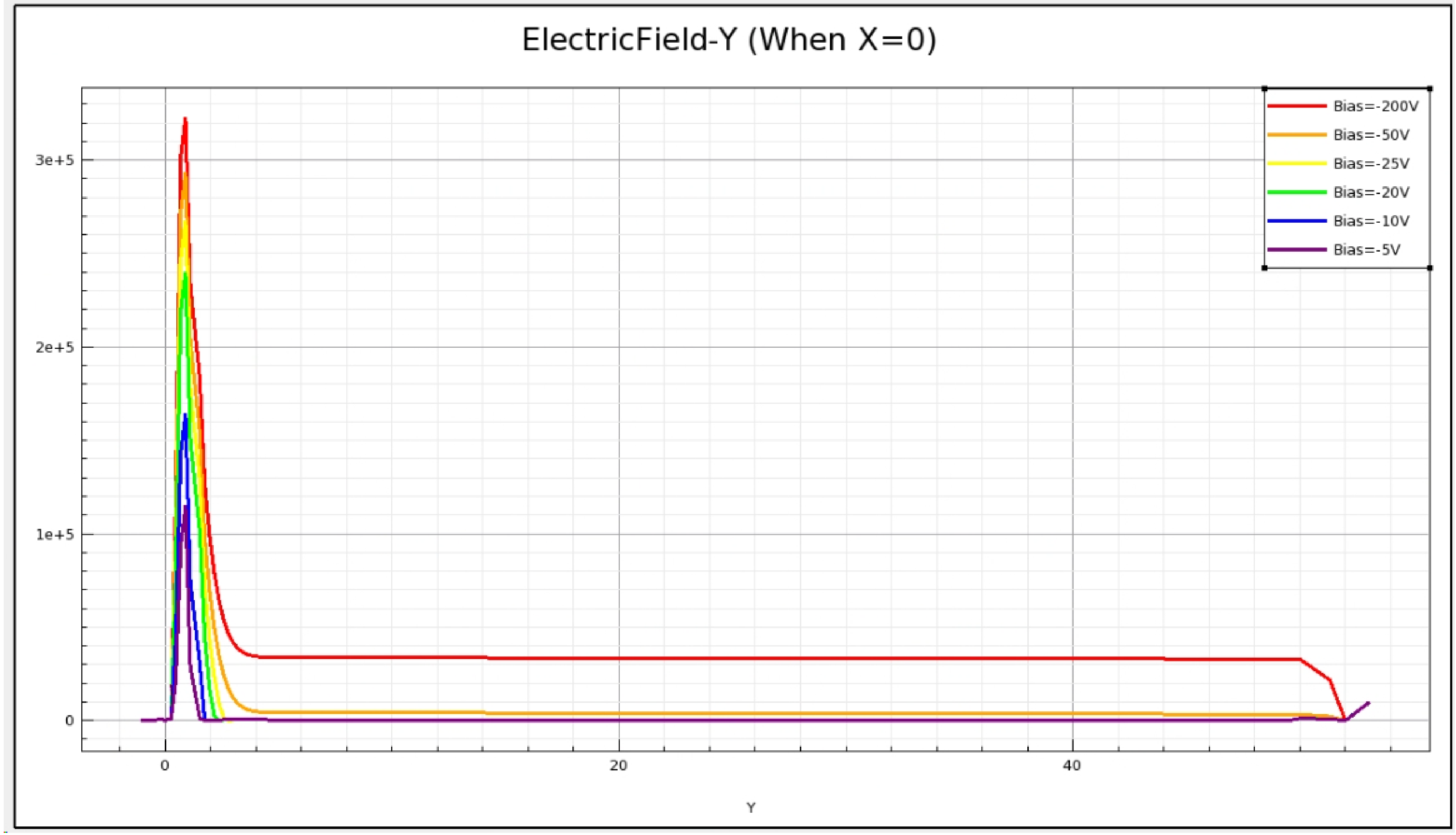
TCAD: ElectricField-V





• Backup

TCAD: ElectricField-V



• Questions and Answers 1

- **1. It is recommended to simulate defect evolution under low-temperature conditions (-30°C), as this is expected to reveal highly interesting phenomena.**

  Thank you for your suggestion. We will take into account the simulation of defect evolution under low-temperature conditions in our subsequent work.

- **2. The diffusion equations considered in the KMC simulations should also be documented.**

  Thank you for your suggestion. The table on the right presents the diffusion equations employed in this KMC simulation.

- **3. Has the influence of the electric field on defect evolution been considered?**

  Thank you for your suggestion. Currently, our KMC simulations are performed under annealing at 300 K without an electric field.

Interaction type	Reaction equation
Self-interstitial / vacancy defects	$I + V \rightleftharpoons 0$ $I + I_n \rightleftharpoons I_2, I_3, I_4, I_5$ (ICluster) $V + V_m \rightleftharpoons V_2, V_3, V_4, V_5$ (VCluster) IVCluster + IVCluster ⇌ IVCluster
Oxygen-related defects	V + Oi ⇌ VOi I + O ⇌ Oi Ci + Oi ⇌ CiOi Bi + Oi ⇌ BiOi
Boron-related defects	B + I ⇌ Bi B + V ⇌ BV Bi + V ⇌ B (or BV + I ⇌ B)
Carbon-related defects	C + I ⇌ Ci Ci +C⇌ CCluster CV + I ⇌ C