Proton-radiation induced vacancies in graphene

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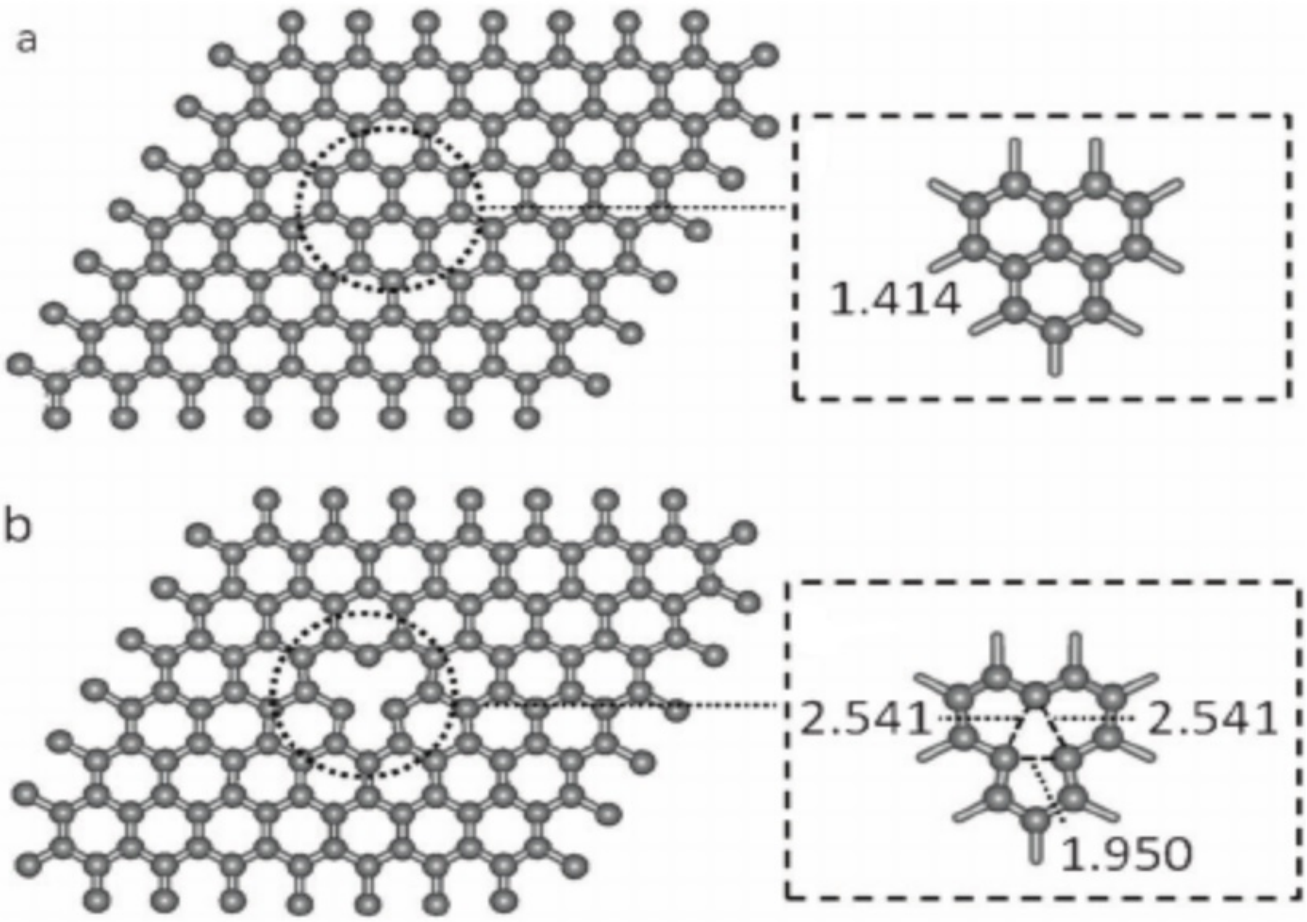
Agenda

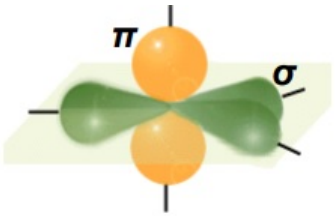
1. Graphene and its properties
2. Interest in the field
3. Model the radiation interaction with graphene
4. Monte Carlo (SRIM) simulation
5. Results

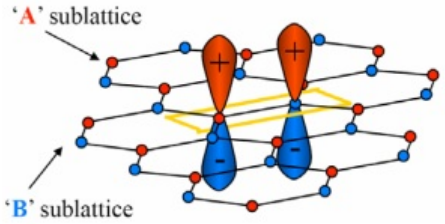
Graphene

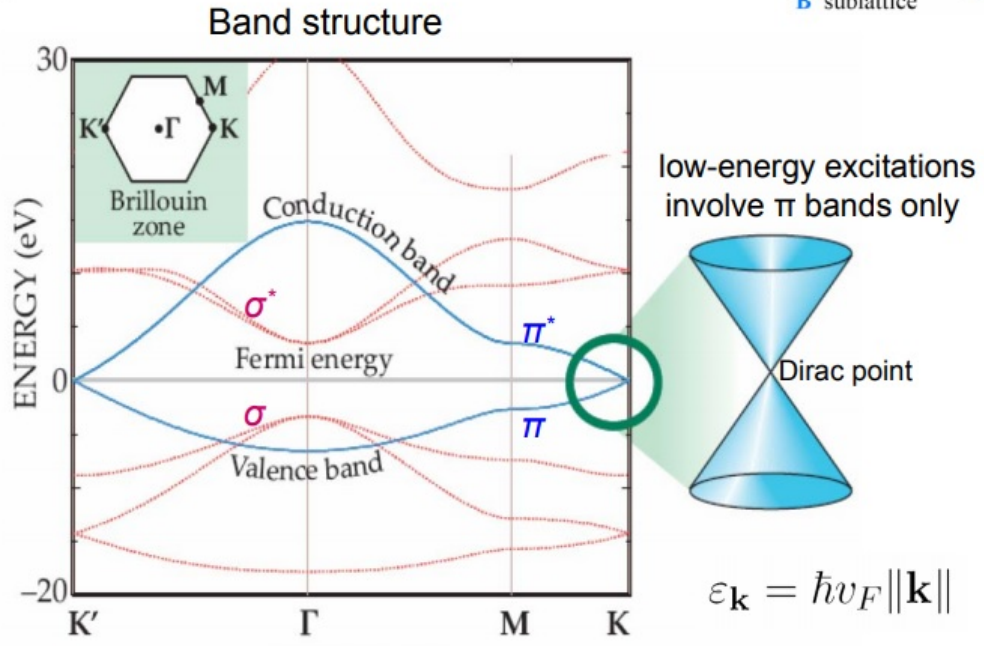


a. Perfect graphene
b. Grapene with a single vacancy

Graphene - properties







- Extremely strong
- Best electrical conductivity
- The perfect graphene has a zero band gap

Interest in the field

- Fundamental interest:

  the well-known cross-sections can not be directly used for interactions in 2D

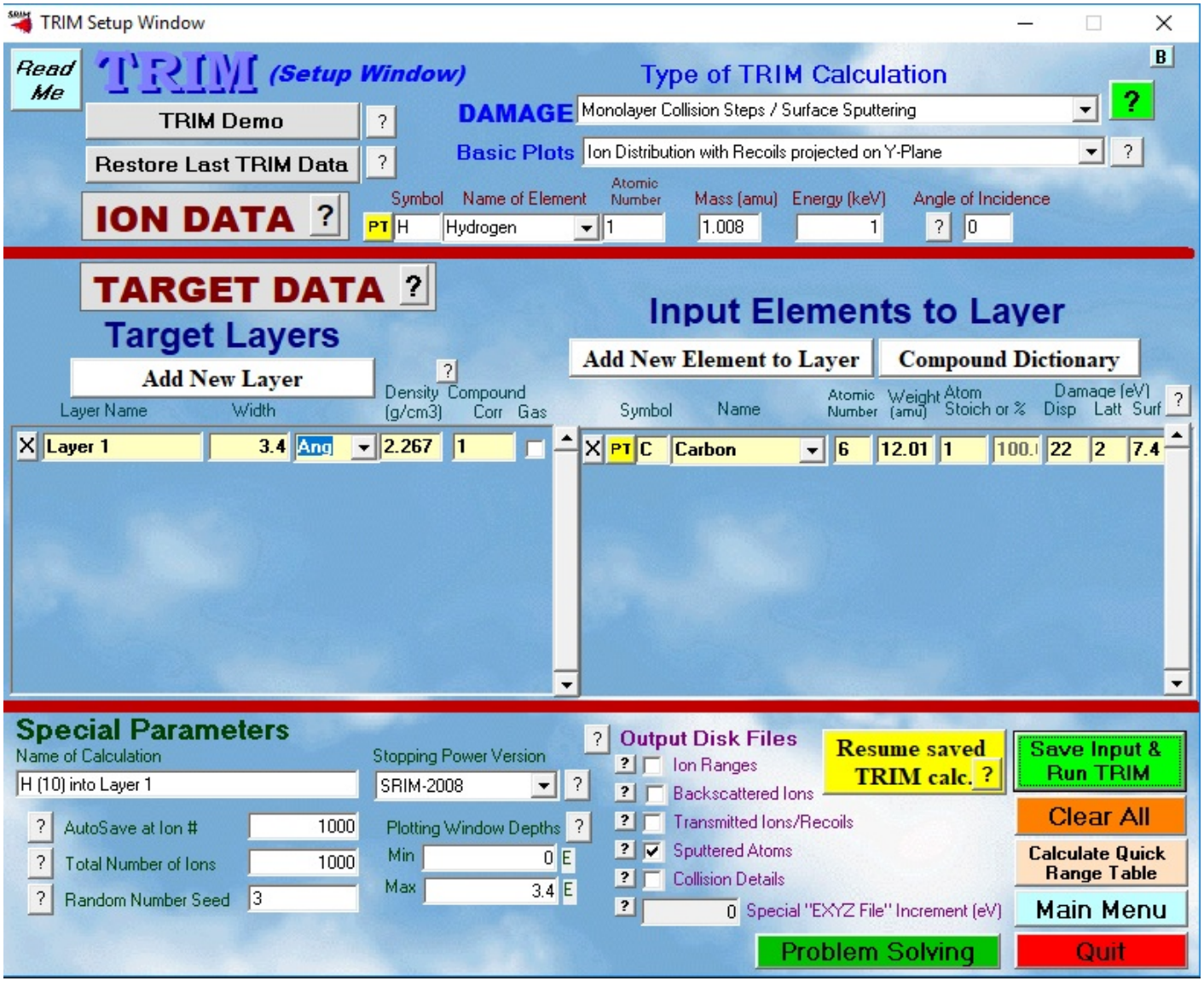
- Practical interest:

  applications in spintronics of graphene with vacancies - controlable

Model the radiation interaction with graphene

- Model of successive, binary interactions.
- No crystal effects causing channeling.
- The polarization of the medium leads to different scattering in the range of collective interactions.
- The ion trajectory is traced until its energy goes under the plasmons excitation energy (2 eV).

TRIM setup


TRIM Setup Window
Read Me
TRIM (Setup Window)
Type of TRIM Calculation
TRIM Demo
DAMAGE
Monolayer Collision Steps / Surface Sputtering
Restore Last TRIM Data
Basic Plots
Ion Distribution with Recoils projected on Y-Plane
ION DATA
Symbol
Name of Element
Atomic Number
Mass (amu)
Energy (keV)
Angle of Incidence
PT H Hydrogen 1 1.008 1 0
TARGET DATA
Target Layers
Add New Layer
Layer Name
Width
Density (g/cm3)
Compound Corr
Gas
Layer 1 3.4 Ang 2.267 1
Input Elements to Layer
Add New Element to Layer
Compound Dictionary
Symbol
Name
Atomic Number
Weight (amu)
Atom Stoich or %
Damage (eV) Disp Latt Surf
PT C Carbon 6 12.01 1 100.0 22 2 7.4
Special Parameters
Name of Calculation
H (10) into Layer 1
Stopping Power Version
SRIM-2008
AutoSave at Ion #
1000
Total Number of Ions
1000
Random Number Seed
3
Plotting Window Depths
Min
0 E
Max
3.4 E
Output Disk Files
Ion Ranges
Backscattered Ions
Transmitted Ions/Recoils
Sputtered Atoms
Collision Details
0 Special "EXYZ File" Increment (eV)
Resume saved TRIM calc.
Save Input & Run TRIM
Clear All
Calculate Quick Range Table
Main Menu
Problem Solving
Quit

Results

Energy [keV]	0.6	0.65	0.7	0.75	0.8	0.9	0.95	1	1.1	1.2	1.3	1.4	1.5	2
Sputtered attoms	10	8	9	10	11	12	12	14	11	16	11	9	11	7

Dependence of the number of sputtered carbon atoms and proton energy. Total number of protons is 1000.

Results

Proton											
Energy [keV]	0.6	0.7	0.8	0.9	1	1.1	1.2	1.3	1.4	1.5	2
Sputtered attoms	89	62	65	62	61	65	58	56	60	70	47

Carbon											
Energy [keV]	0.6	0.7	0.8	0.9	1	1.1	1.2	1.3	1.4	1.5	2
Sputtered attoms	1460	1423	1430	1384	1347	1347	1395	1350	1332	1317	1331

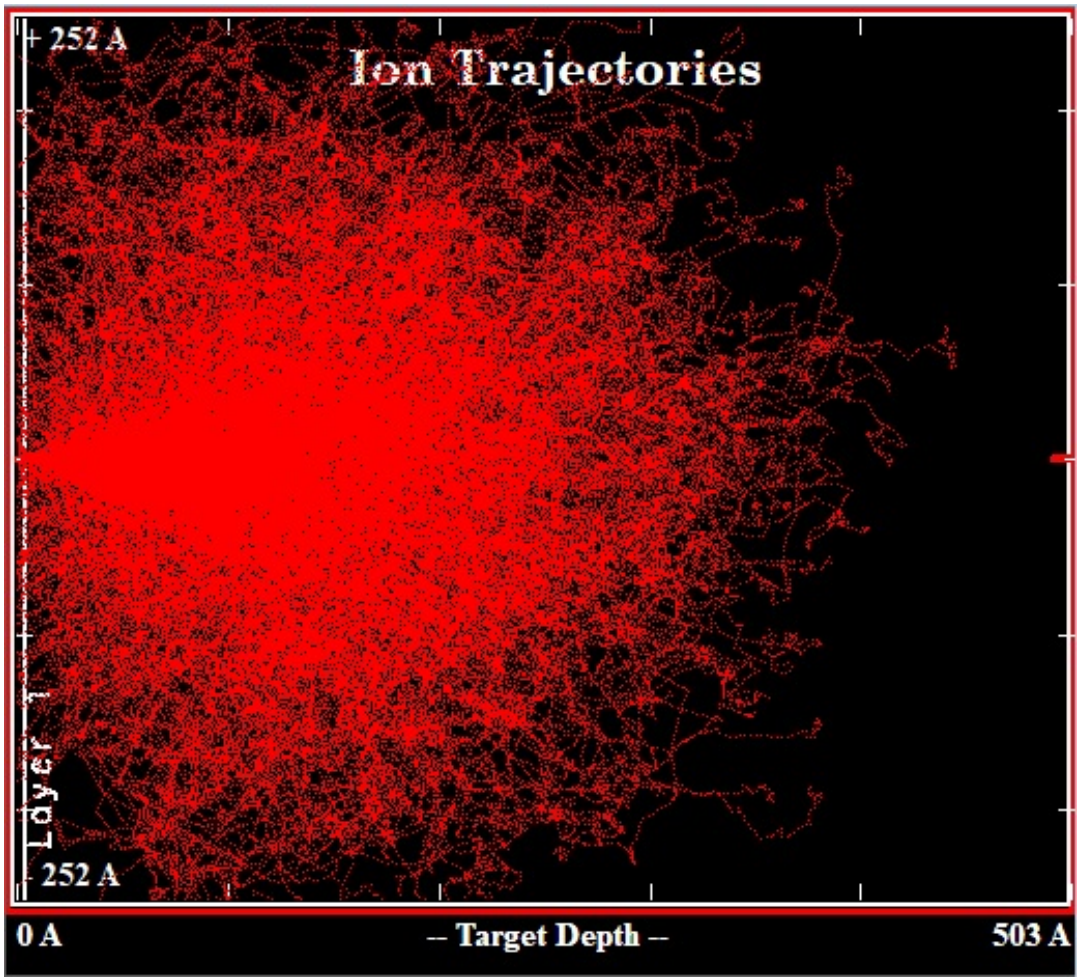
Relation between number of sputtered atoms and proton / carbon ion energy. Total number of ions is 1000.

Results

Energy [MeV]	Defect yield	SiO2		Graphene	
		Sn (keV/nm)	Se (keV/nm)	Sn (keV/nm)	Se (keV/nm)
1	0.007	0.0092	1.06	0.0097	1.35
3	0.004	0,0039	1.44	0.0034	1.77

Defect yield in SiO2-supported graphene, nuclear stopping power (Sn) and electronic stopping power (Se) under irradiation with a carbon ion beam.

Results



Total number of protons = 1000

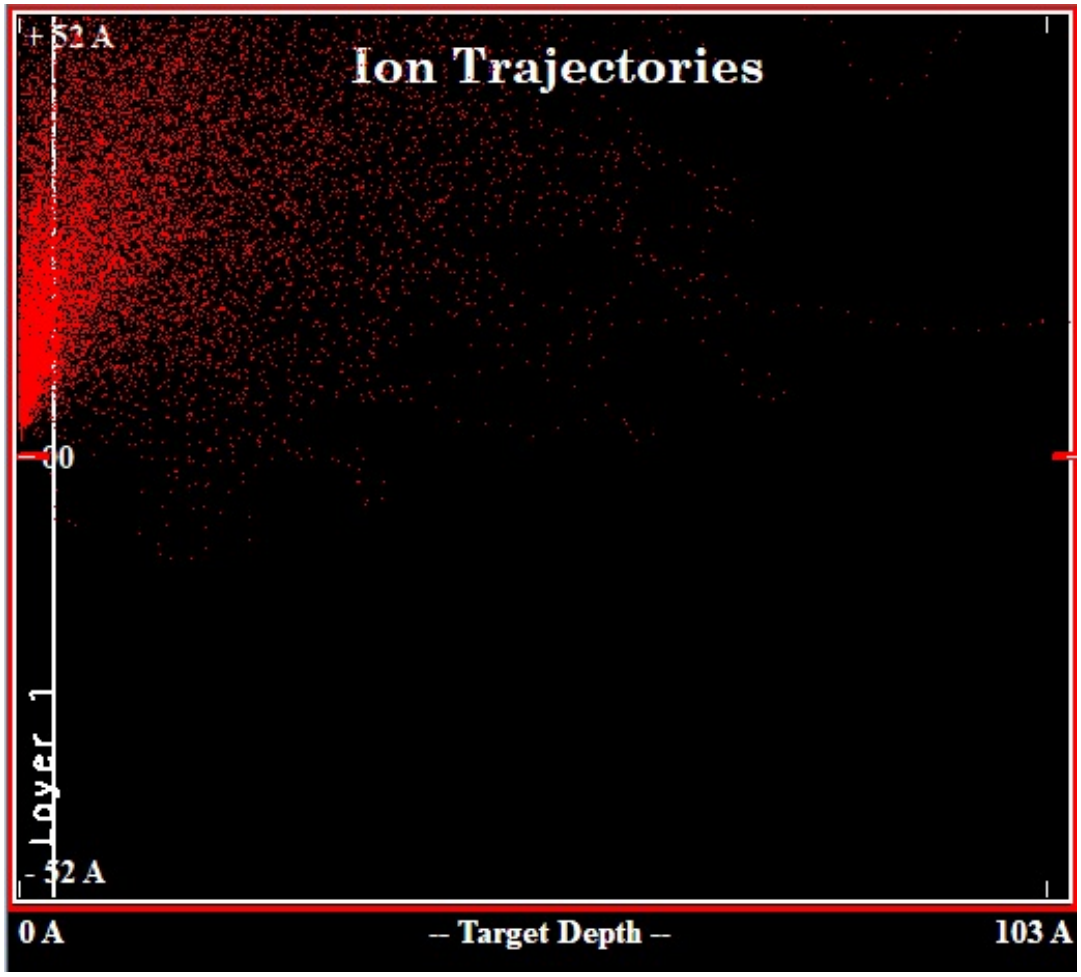
Energy [eV] = 800 eV

Angle = 90 deg

Sputtered atoms = 8

Sputtered atoms (with SiO2) = 10

Results



Total number of protons = 1000

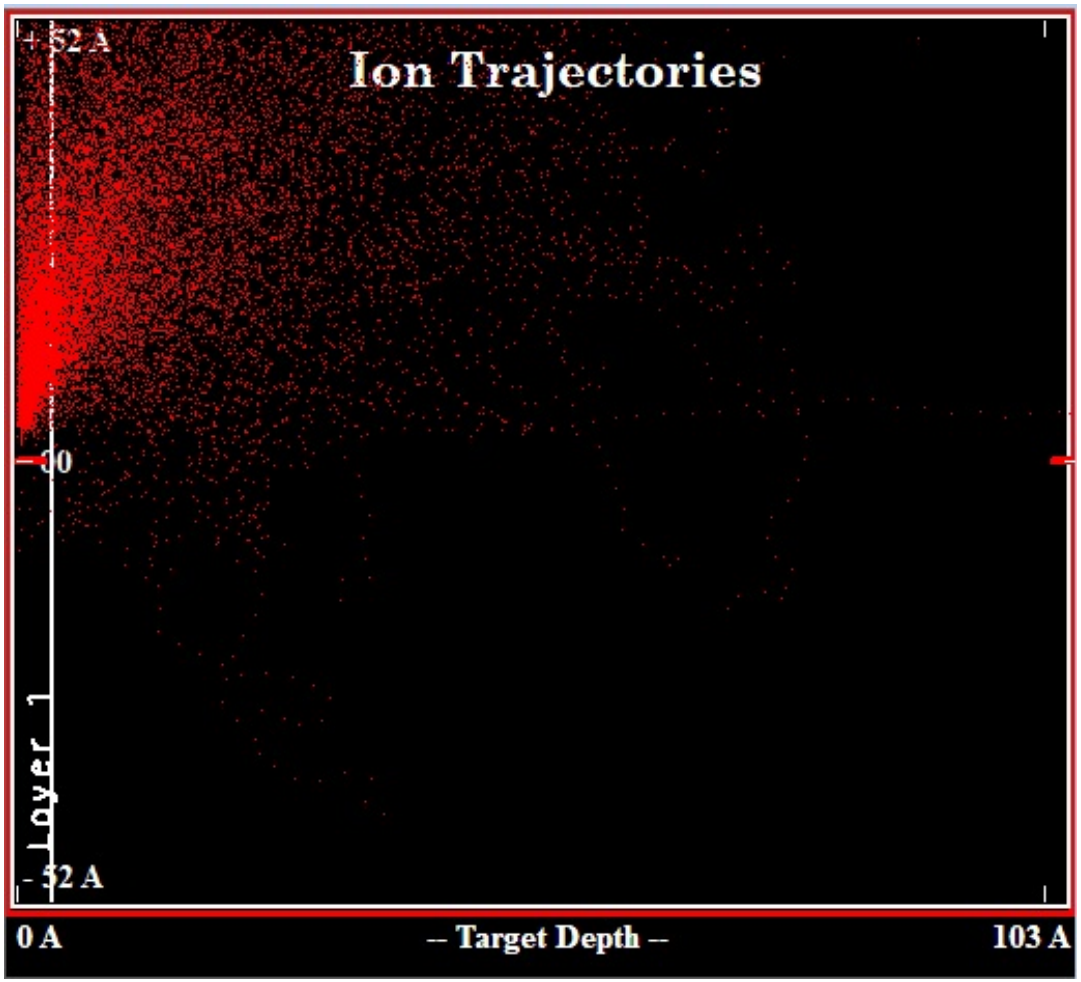
Energy [eV] = 800 eV

Angle = 5 deg

Sputtered atoms = 73

Sputtered atoms (with SiO2) = 118

Results



Total number of protons = 1000

Energy [eV] = 800 eV

Angle = 10 deg

Sputtered atoms = 57

Sputtered atoms (with SiO2) = 104

Results

- Larger number of atoms are knocked out when beam falls at a smaller angle to the surface.

- For generating a very small number of vacancies, the beam should be perpendicular to the surface, with an optimal range of energy 600 eV – 2 keV.

- SRIM results agree with the expected number of generated vacancies, depending on the energy and intensity of the proton beam.

References

[1] Dobrina Borisova, Vladislav Antonov, Ana Proykova, https://doi.org/10.1002/qua.24077

[2] James F.Ziegler, SRIM The Stopping and Range of Ions in Matter, ISBN-13: 978-0-9654207-1-6, 2008

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Thank you for your attention!