Crystal lattice defects induced by swift heavy ions in 3C-SiC: study of repair mechanisms at high temperatures

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New reactor concepts and safety analyses for the Polish Nuclear Energy Program
POWR.03.02.00-00.I005/17

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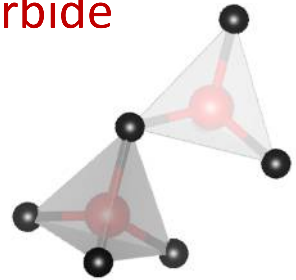
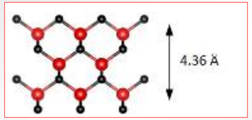
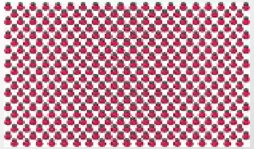
- Silicon Carbide
- Ion irradiation damage
- Si and C ion irradiation of SiC – experimental results
- MD simulations of low energy ion irradiation
- Thermal Spike model
- MD simulation of TS model
- Conclusion

Silicon Carbide

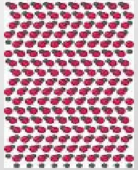




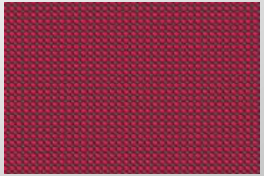
Monocrystal 3C-SiC



6H-SiC

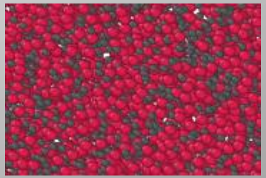


Monocrystal 3C-SiC



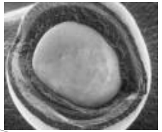
Polycrystal SiC

Amorphous SiC



Silicon Carbide application

NUCLEAR

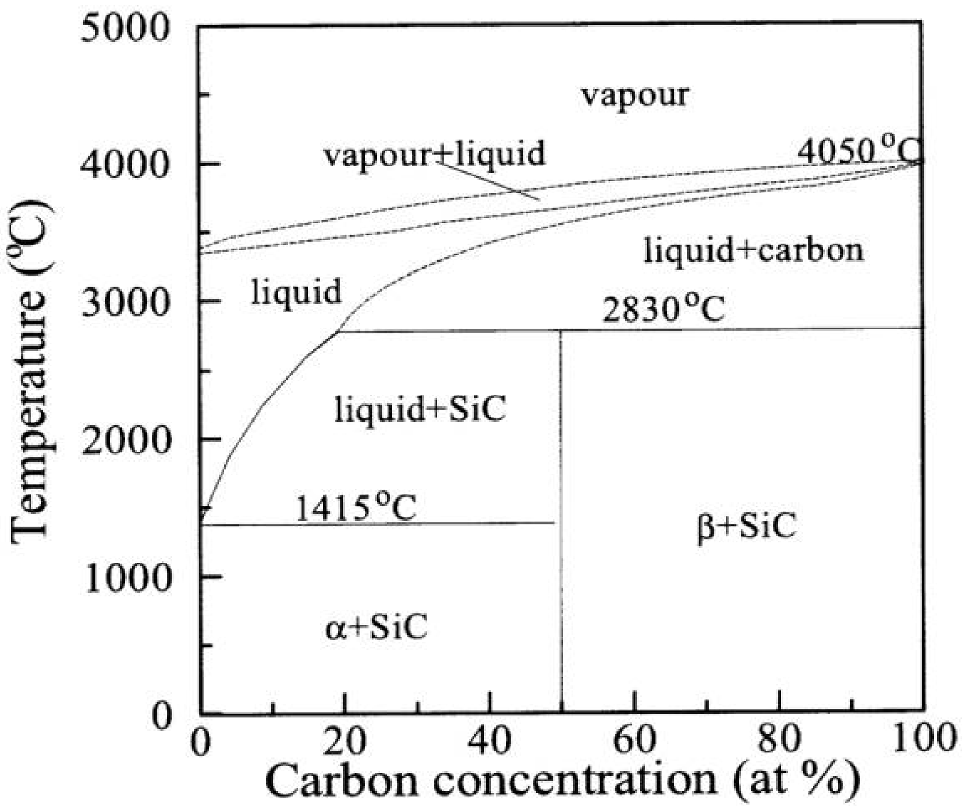


SPACE

ELECTRONIC

http://xqprevention.com/silicon-carbide-3.html
https://www.ga.com/nuclear-fission/siga-sic-composite
https://en.wikipedia.org/wiki/ITER#/media/File:ITER_Exhibit_(01810402)_(12219071813)_(cropped).jpg
https://www.energy.gov/ne/articles/triso-particles-most-robust-nuclear-fuel-earth
https://www.mersen.com/products/graphite-specialties/boostecr-silicon-carbide-sic/space-and-astronomy
https://ntts-prod.s3.amazonaws.com/t2p/prod/t2media/tops/pdf/LEW-TOPS-131.pdf

Silicon Carbide



https://trace.tennessee.edu/cgi/viewcontent.cgi?referer=&httpsredir=1&article=3115&context=utk_chanhonoproj

Ion radiation damage

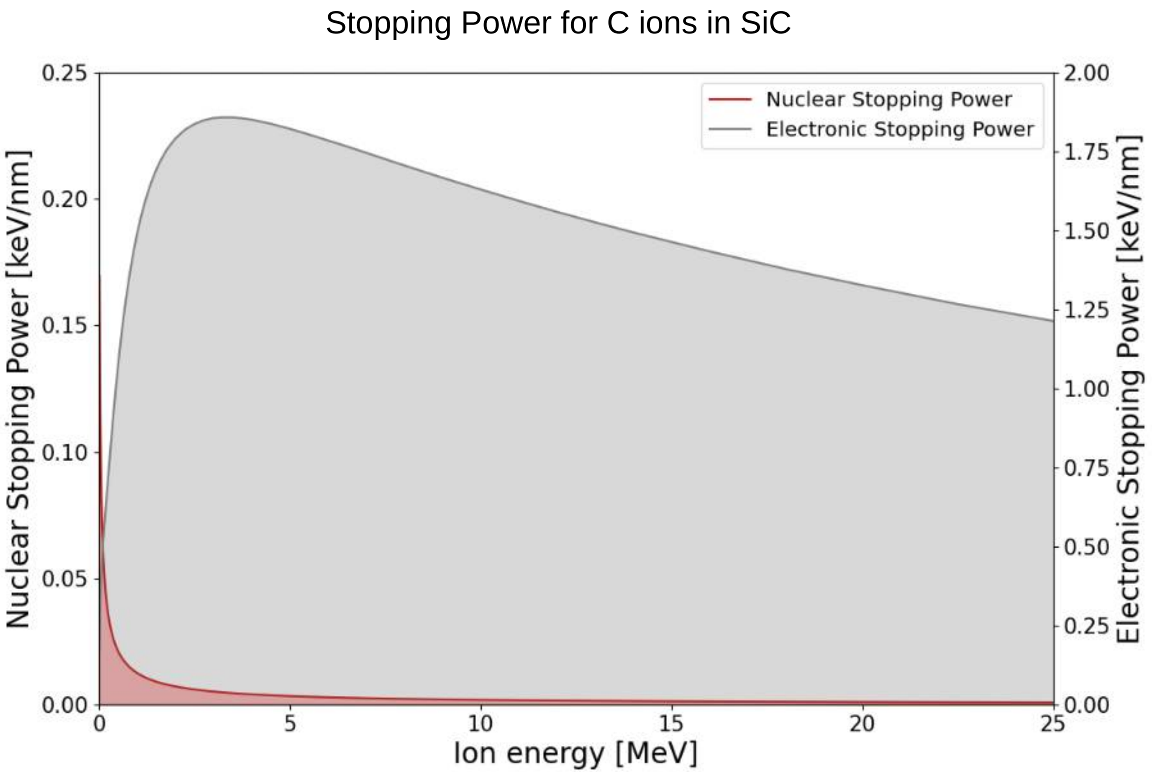
Energetic incident ions lose their energy through two different energy processes:

→ Nuclear energy loss

the transfer of kinetic energy occurs via elastic scattering

→ Electronic energy loss

the inelastic transfer of energy to electrons (i.e. ionization and excitation)



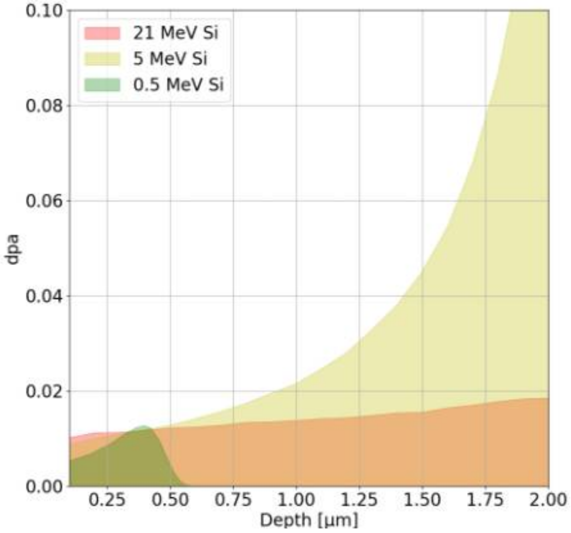
Displacement per atom

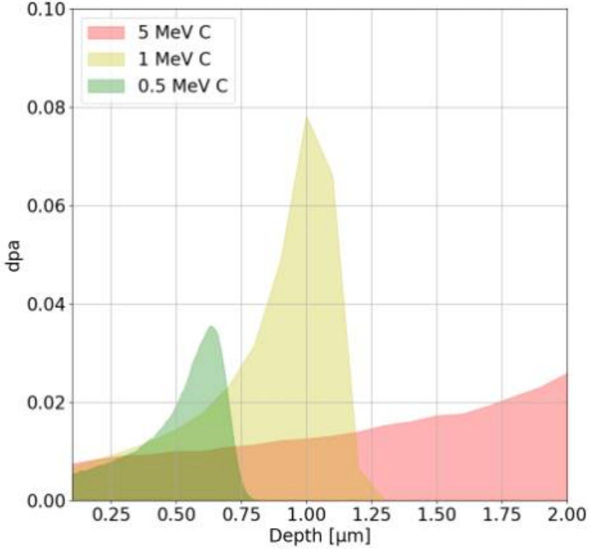
- **Atomic displacements per atom (dpa)** is unit of radiation damage exposure
- The current international standard definition for dpa is based on the Norgett-Robinson Torrens (NRT) model that convert a known value of the damage energy into a corresponding number of atomic displacements
- **The Norgett–Robinson–Torrens model:**

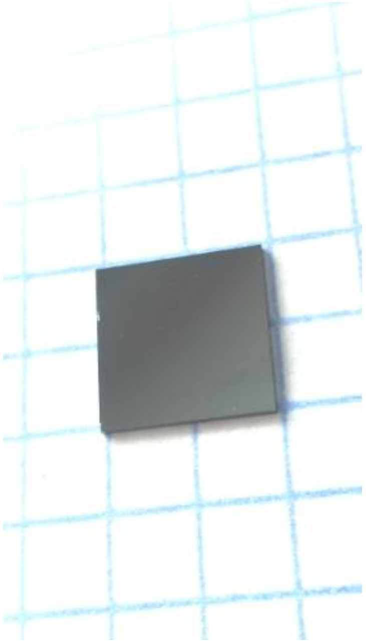
$$\upsilon_{NRT} = \frac{0.8T_d}{2E_d}$$

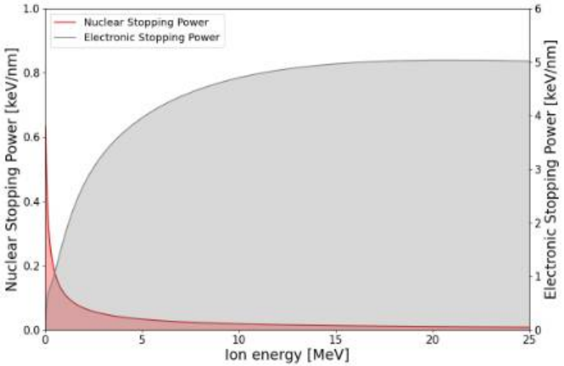
T_d - damage energy,
E_d - displacement energy,

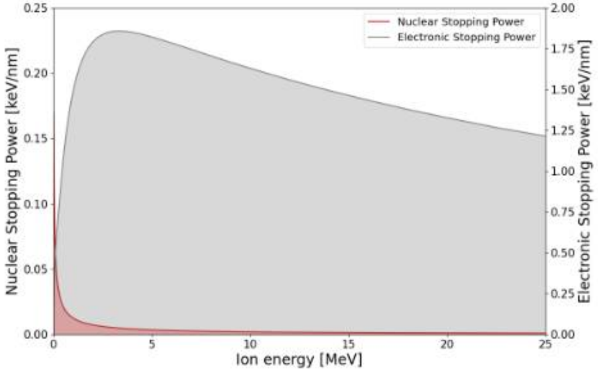
Si and C ions irradiation of SiC



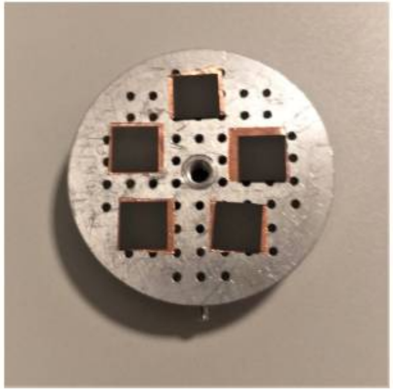


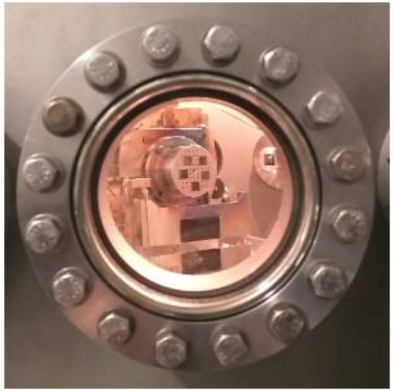


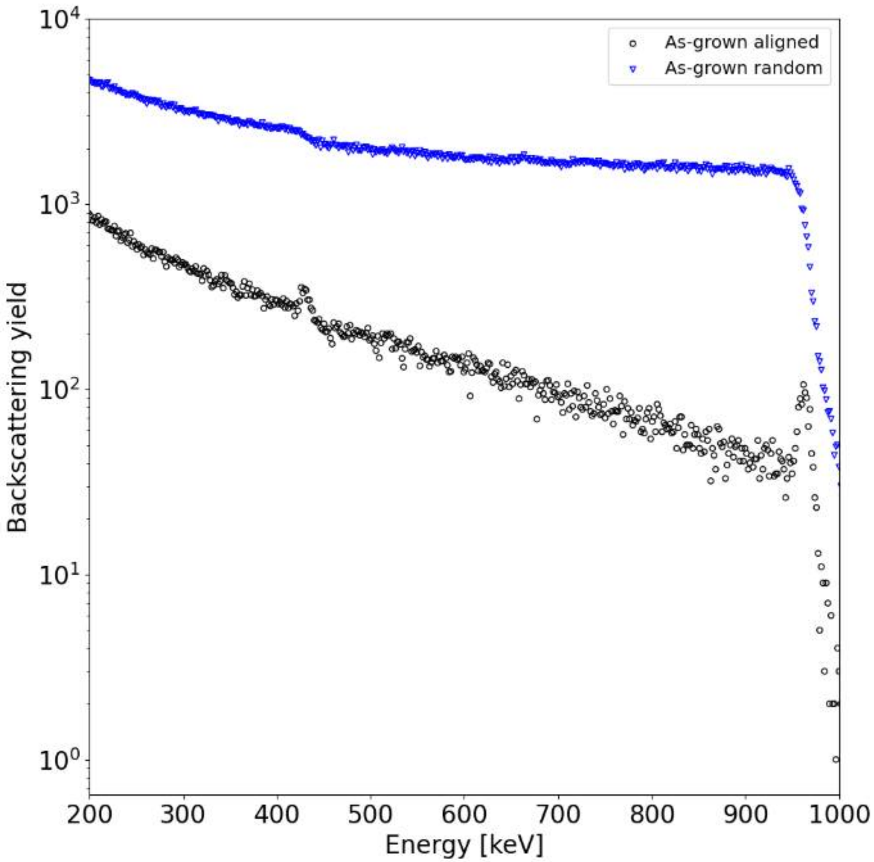




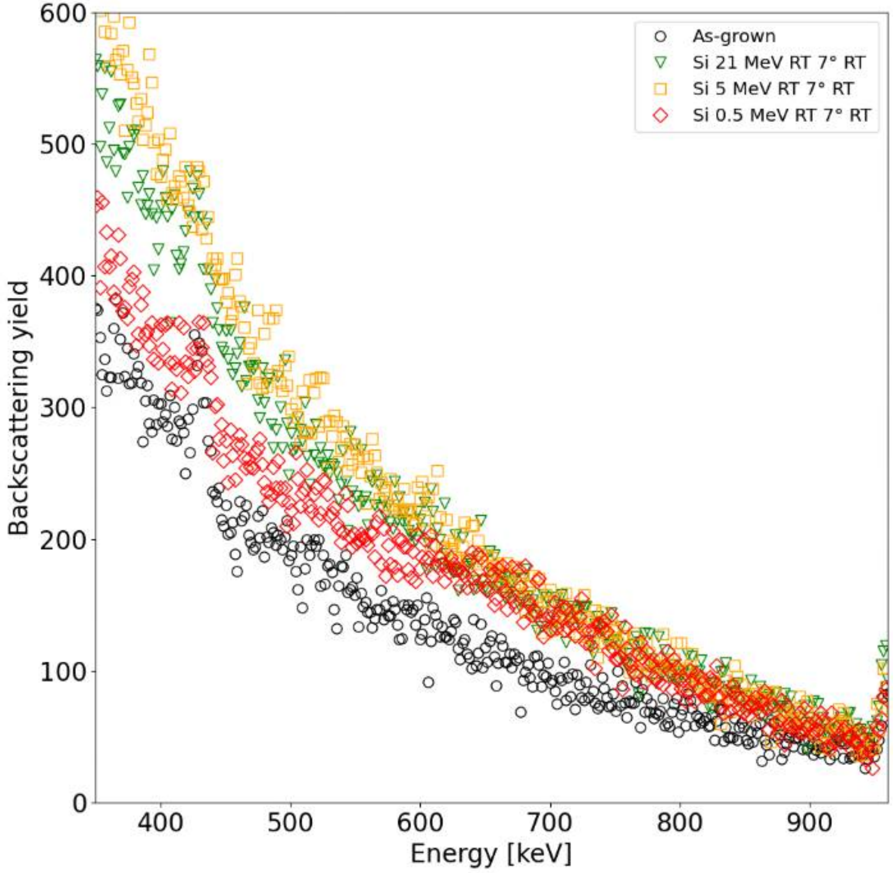
Rutherford Backscattering Spectrometry analysis

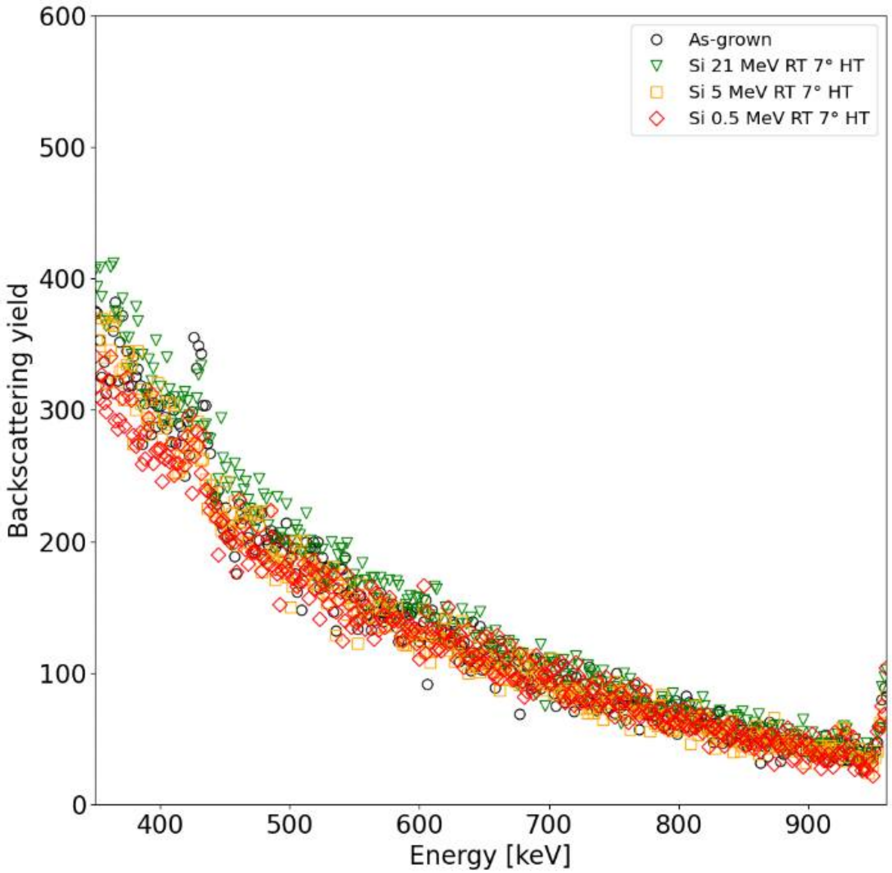




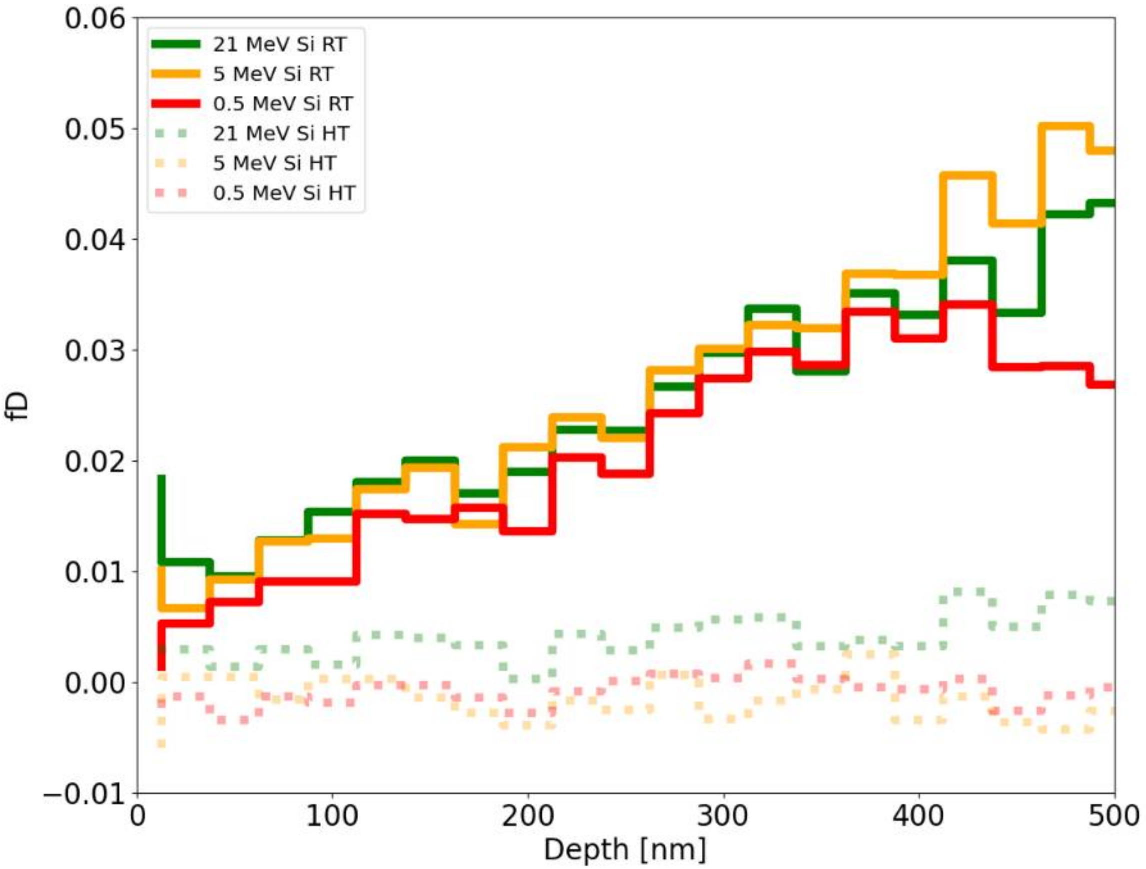


Rutherford Backscattering Spectrometry analysis





Relative defect fraction



Relative defect farction:

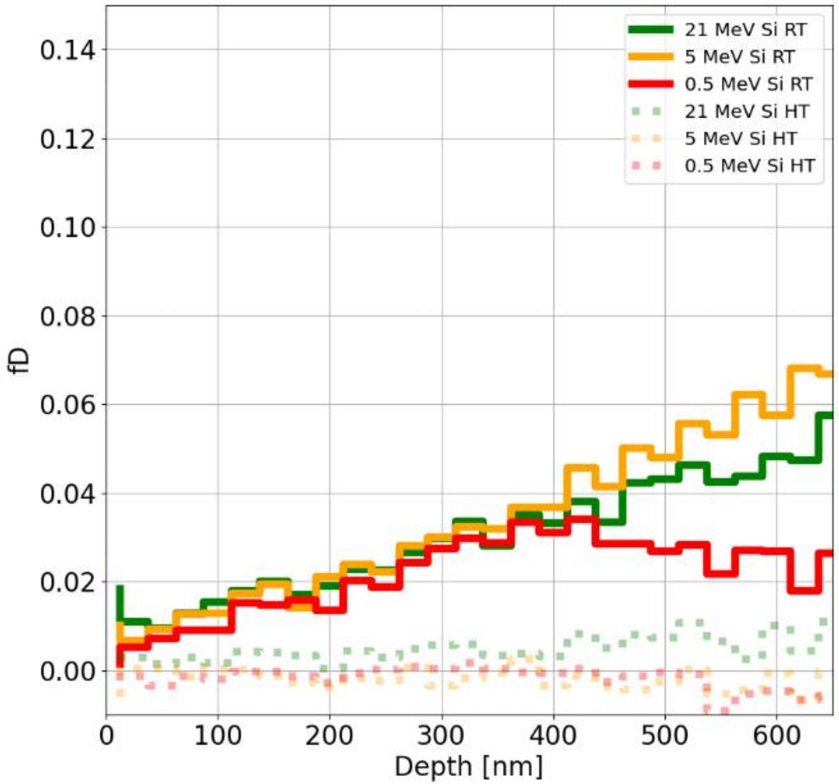
$$f_D = \frac{Y^{irradiated}_{aligned} - Y^{as-grown}_{aligned}}{Y_{random}}$$

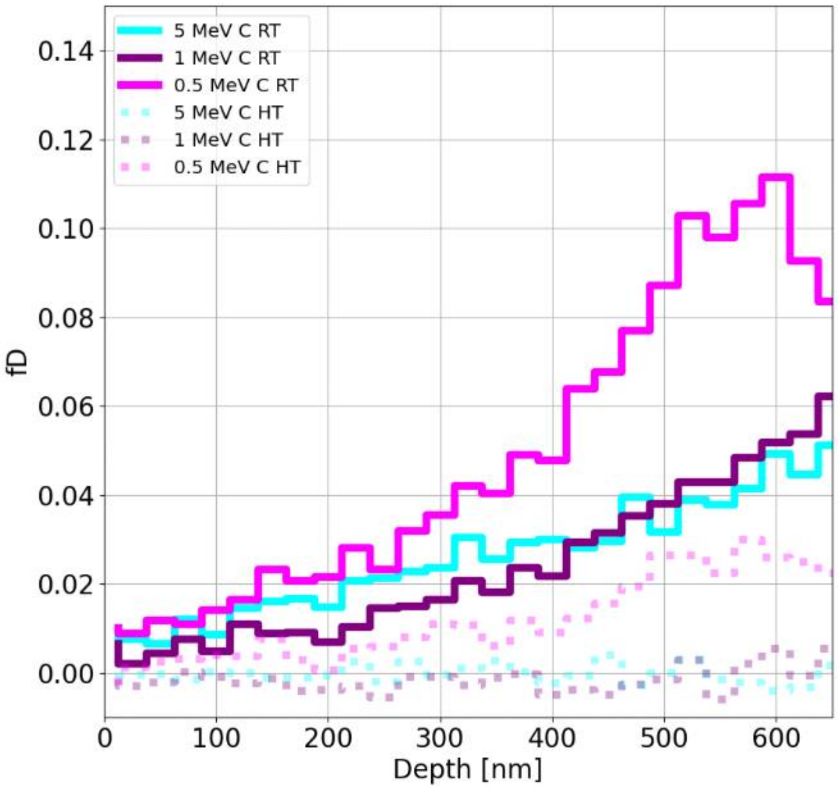
$Y^{irradiated}_{aligned}$ Yield of the irradiated sample

$Y^{as-grown}_{aligned}$ Yield of the as-grown sample

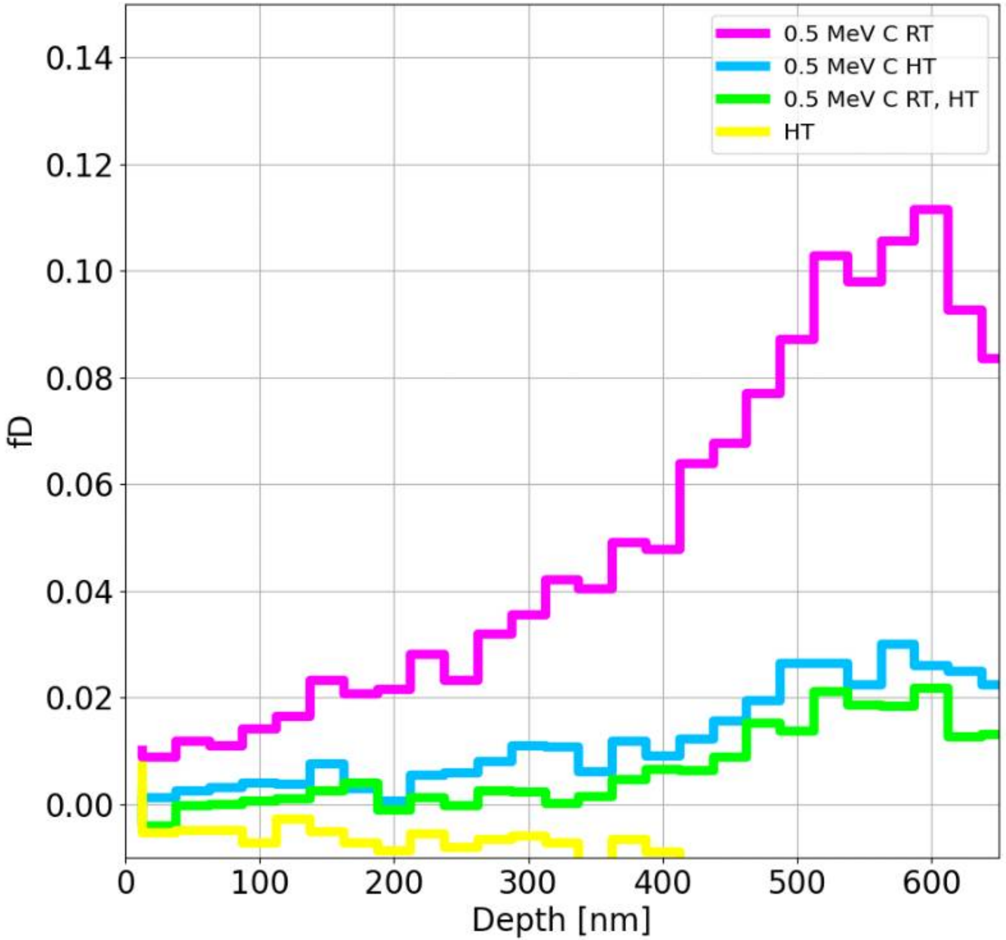
Y_{random} Random Yield

Relative defect fraction

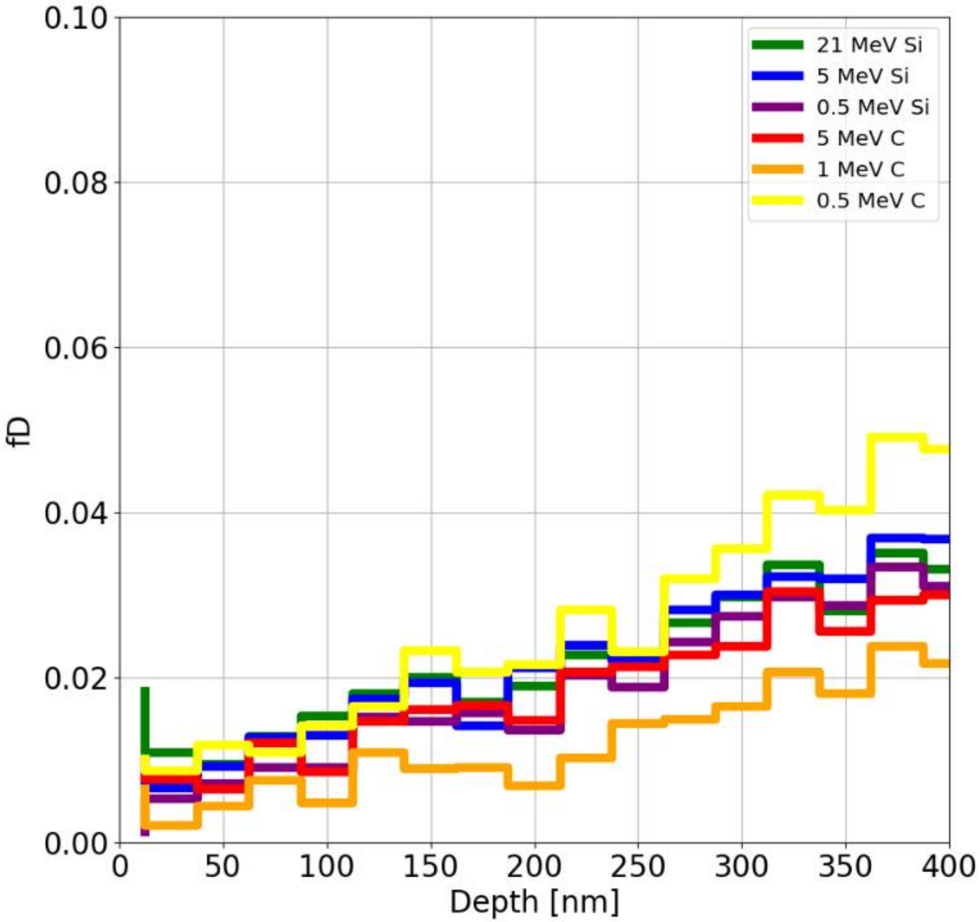


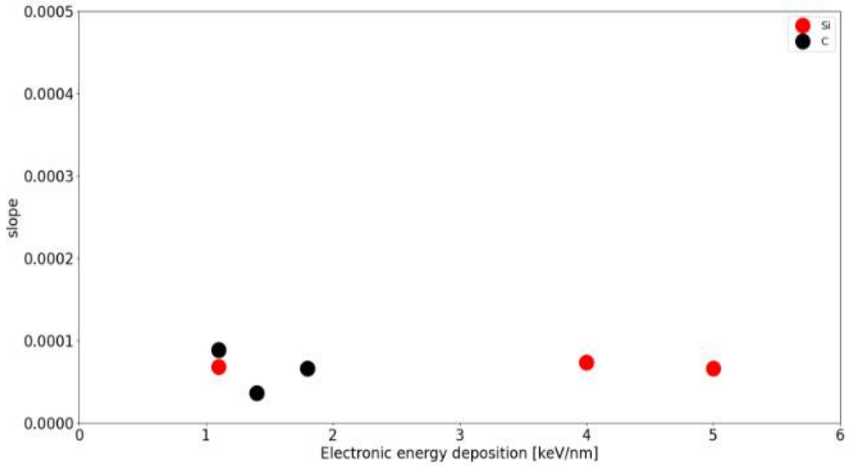


Relative defect fraction



Relative defect fraction

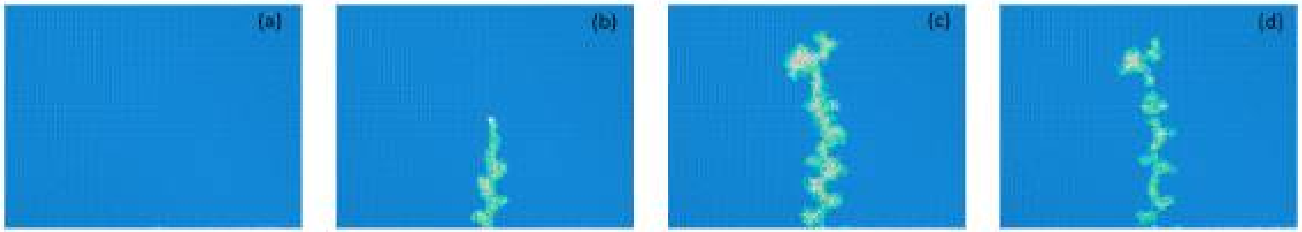




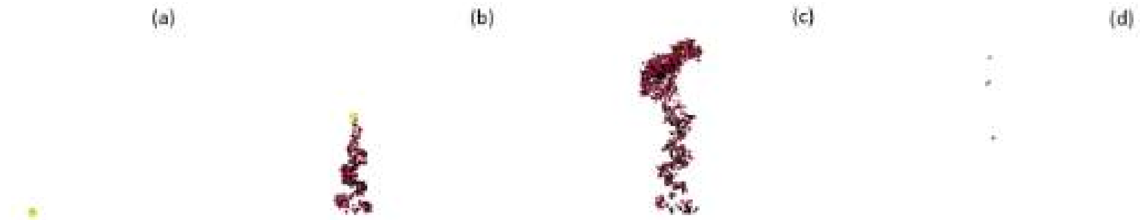
Molecular dynamic simulations

Simulation of 5keV Ar ion irradiation of SiC at time: (a) 0 ps, (b) 0.06 ps, (c) 0.2 ps, (d) 3.2 ps

Crystal Stucture damage



Atoms with kinetic energy > 0.5 eV



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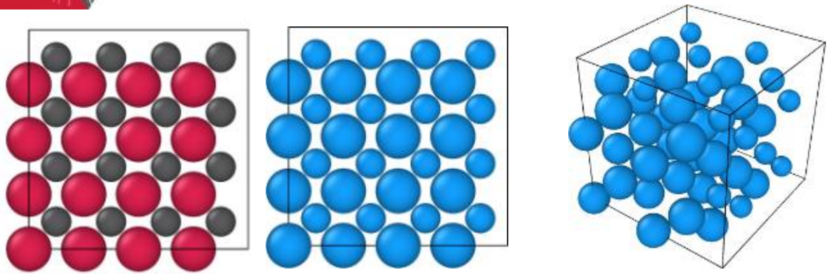
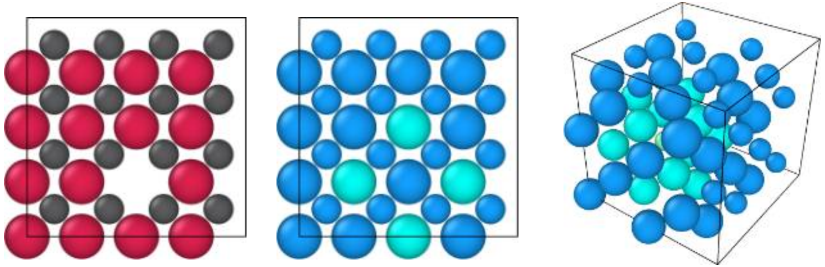
Ovito analysis



Cluster analysis (cutoff: 2):
0 cluster

WS analysis:
0 vacancies
0 interstitials

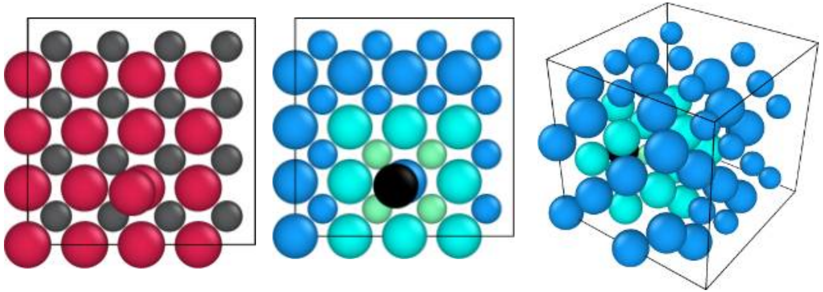
Color	Structure	Count	Fraction	Id
	Other	0	0.0%	0
	Cubic diamond	64	100.0%	1
	Cubic diamond (1st neighbor)	0	0.0%	2
	Cubic diamond (2nd neighbor)	0	0.0%	3



Cluster analysis (cutoff: 2):
1 cluster

WS analysis:
1 vacancies
0 interstitials

Color	Structure	Count	Fraction	Id
	Other	0	0.0%	0
	Cubic diamond	47	74.6%	1
	Cubic diamond (1st neighbor)	12	19.0%	2
	Cubic diamond (2nd neighbor)	4	6.3%	3



Cluster analysis (cutoff: 2):
1 cluster

WS analysis:
1 vacancies
1 interstitials

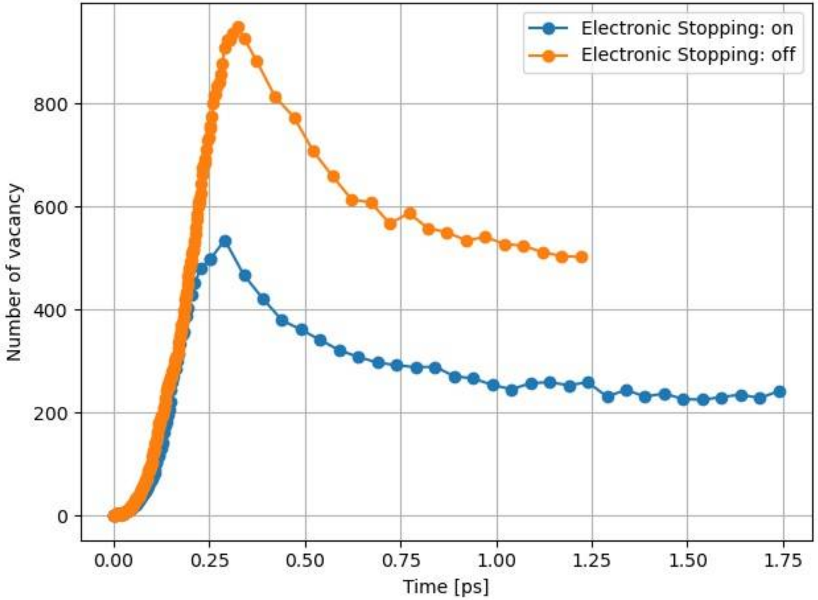
Color	Structure	Count	Fraction	Id
	Other	1	1.6%	0
	Cubic diamond	47	73.4%	1
	Cubic diamond (1st neighbor)	12	18.8%	2
	Cubic diamond (2nd neighbor)	4	6.3%	3

Electronic Stopping Power in MD simulations

- Fix electron/stopping implements inelastic energy loss for fast ions in solids
- It applies a friction force to fast moving atoms to slow them down due to electronic stopping

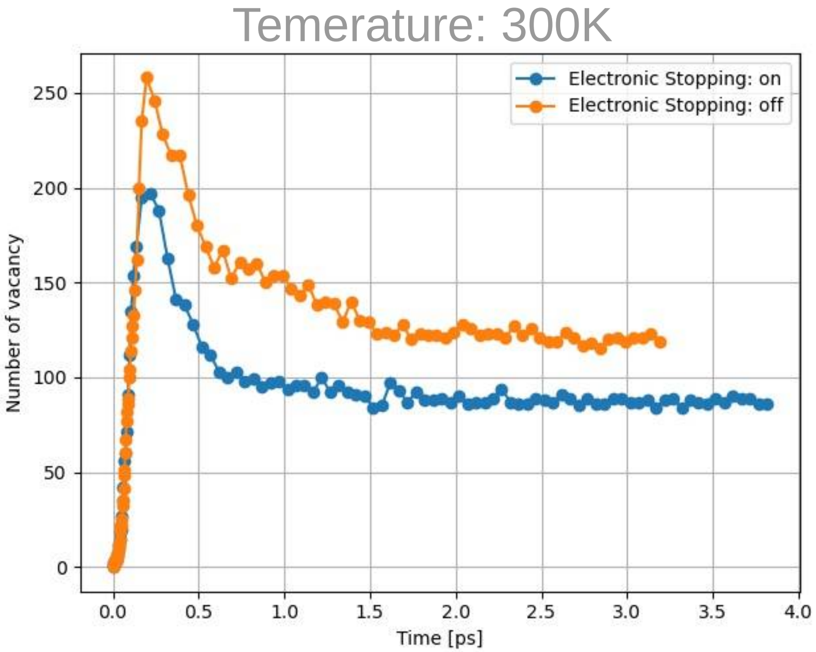
$$m_i \frac{\partial \mathbf{v_i}}{\partial t} = \mathbf{F_i}(t)$$

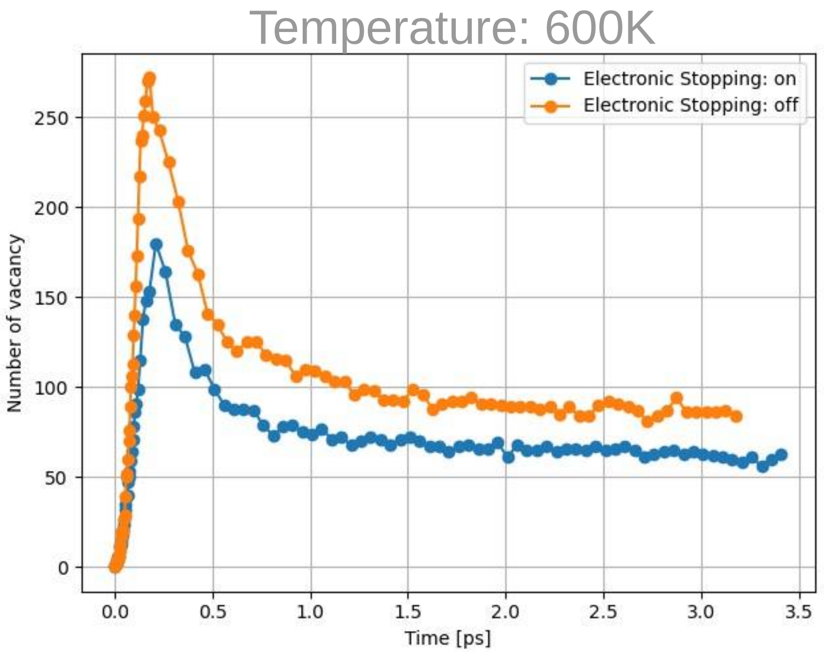
$$m_i \frac{\partial \mathbf{v_i}}{\partial t} = \mathbf{F_i}(t) - \frac{\mathbf{v_i}}{|\mathbf{v_i}|} S_e$$



Ar ion irradiation of SiC (20 keV)

Number of vacancies produced during the 5 keV Ar cascades





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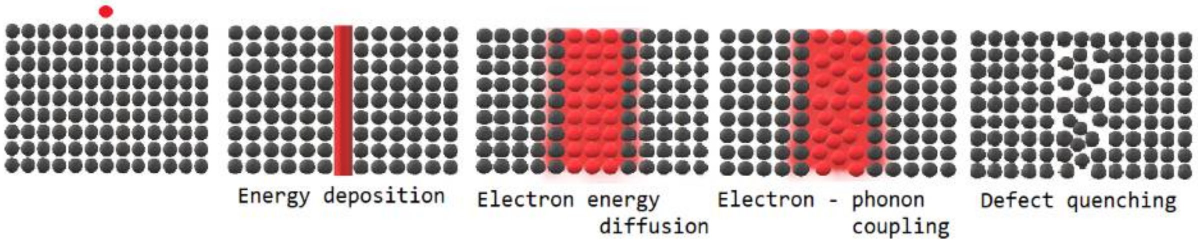
Thermal Spike

The heat diffusion in the electron and lattice subsystems can be described by two coupled differential equations governing the energy diffusion on the electron and atomic subsystems and their exchange via the electron-phonon coupling

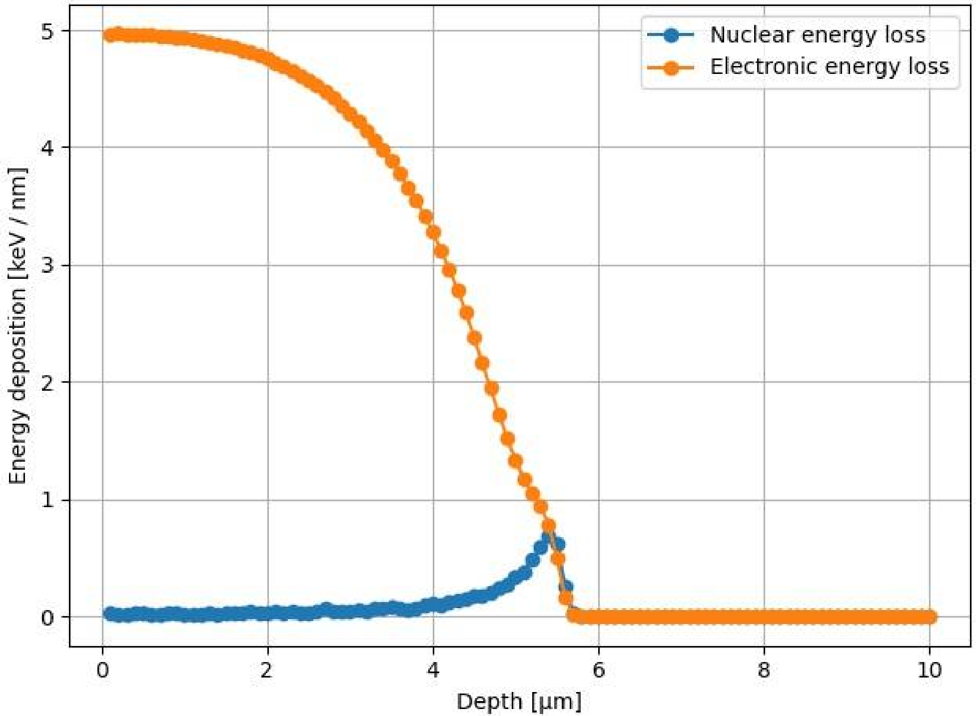
$$C_e(T_e)\frac{\partial T_e}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[rK_e(T_e)\frac{\partial T_e}{\partial r}\right] - g(T_e - T_a) + A(r,t)$$

$$C_a(T_a)\frac{\partial T_a}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[rK_a(T_a)\frac{\partial T_a}{\partial r}\right] + g(T_e - T_a)$$



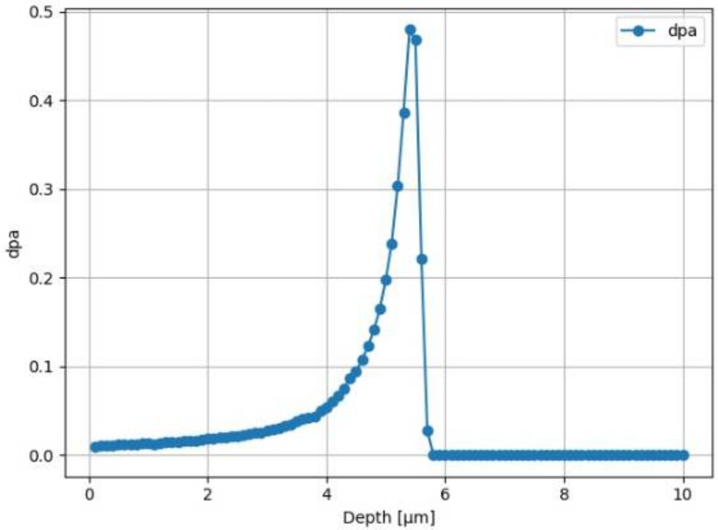
Energy deposition & dpa calculation with using TRIM

21 MeV Si ion in Silicon Carbide



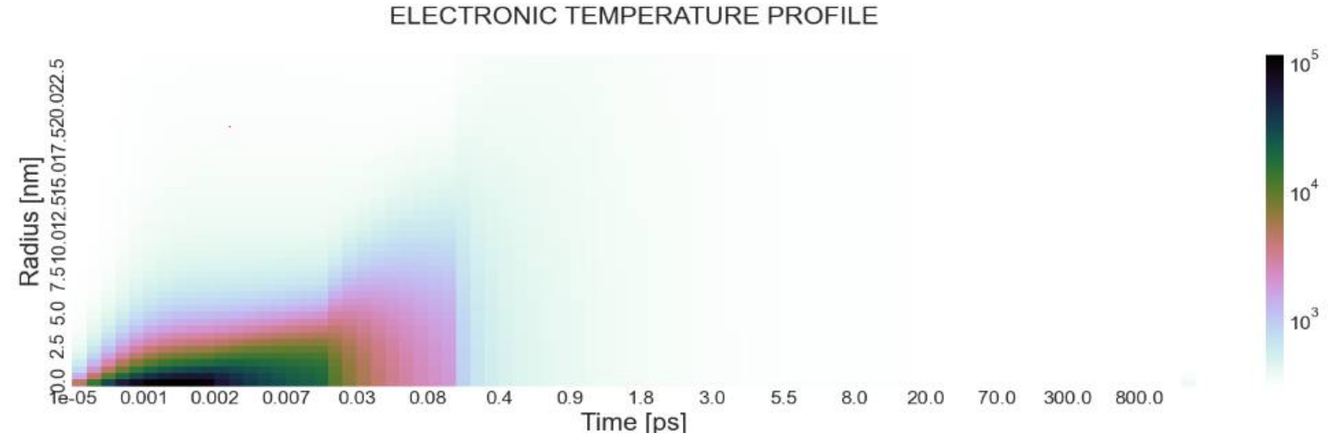
$$\left[\frac{i-v \quad pairs}{nm \cdot ion}\right] => [dpa]$$

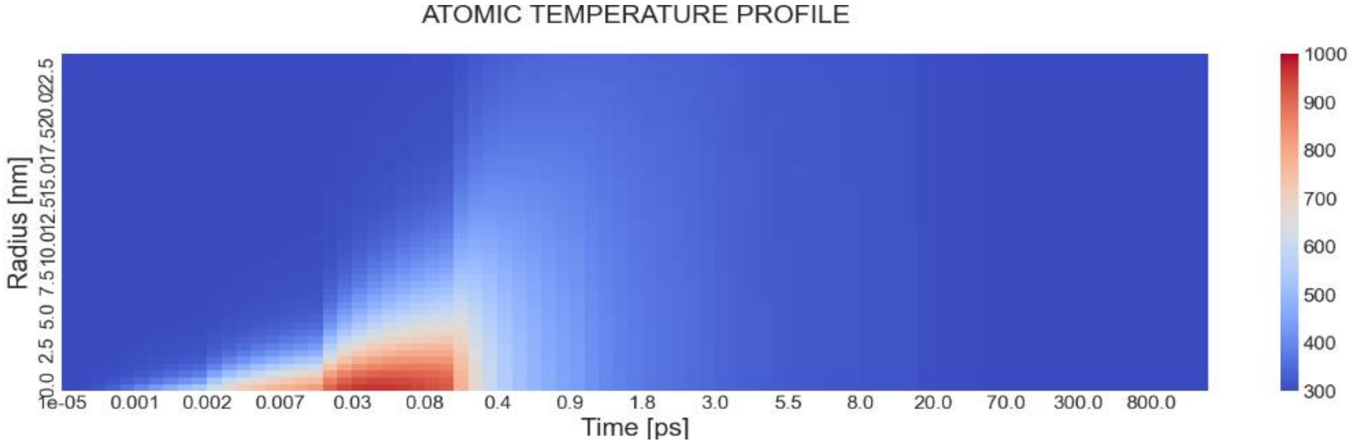
$$\left[\frac{i-v \quad pairs}{nm \cdot ion}\right] \frac{1}{10^{-7}\frac{cm}{nm}} \frac{\phi[\frac{ions}{cm^2}]}{\rho_a[\frac{atoms}{cm^3}]} = \left[\frac{displacements}{atom}\right] = [dpa]$$

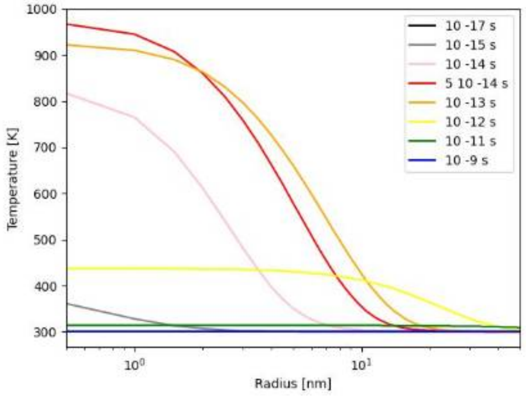


21 MeV Si ion irradiation of SiC

Results from
Thermal Spike 2.15 Gui code
(TS code developed by
C. Dufour, J. Rangama, M. Toulemonde)







Thermal Spike

Results from
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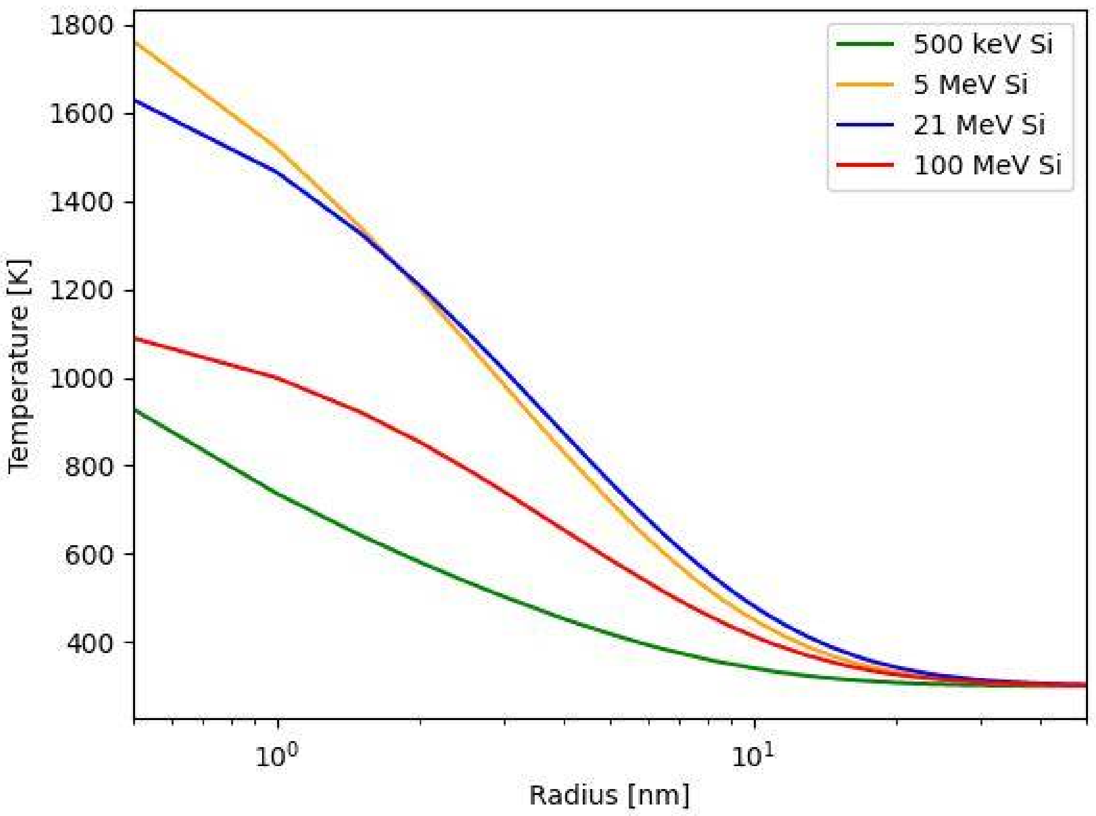
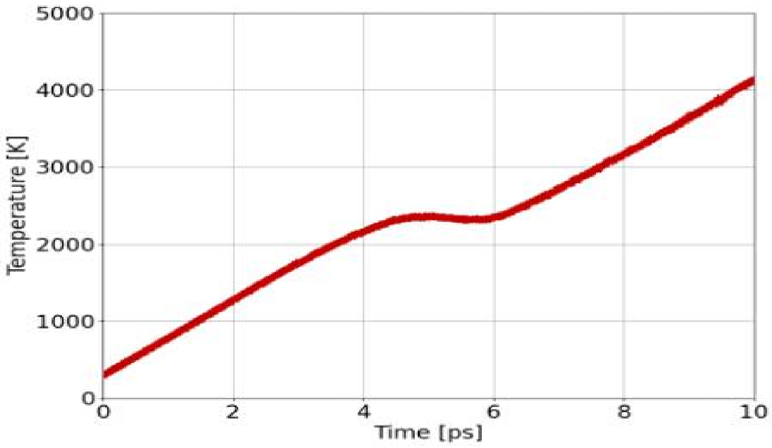
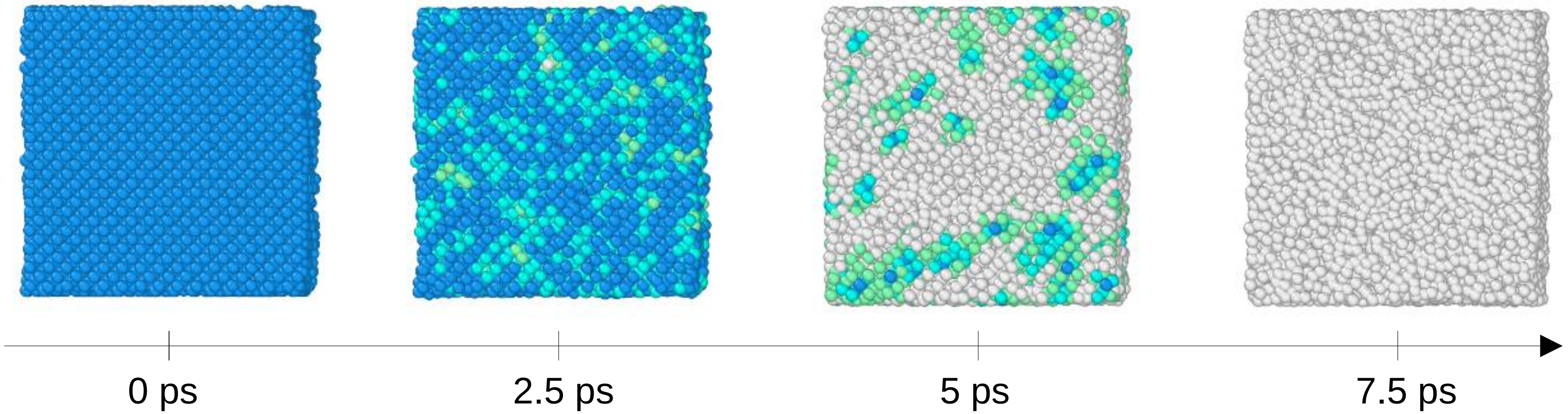


SiC melting

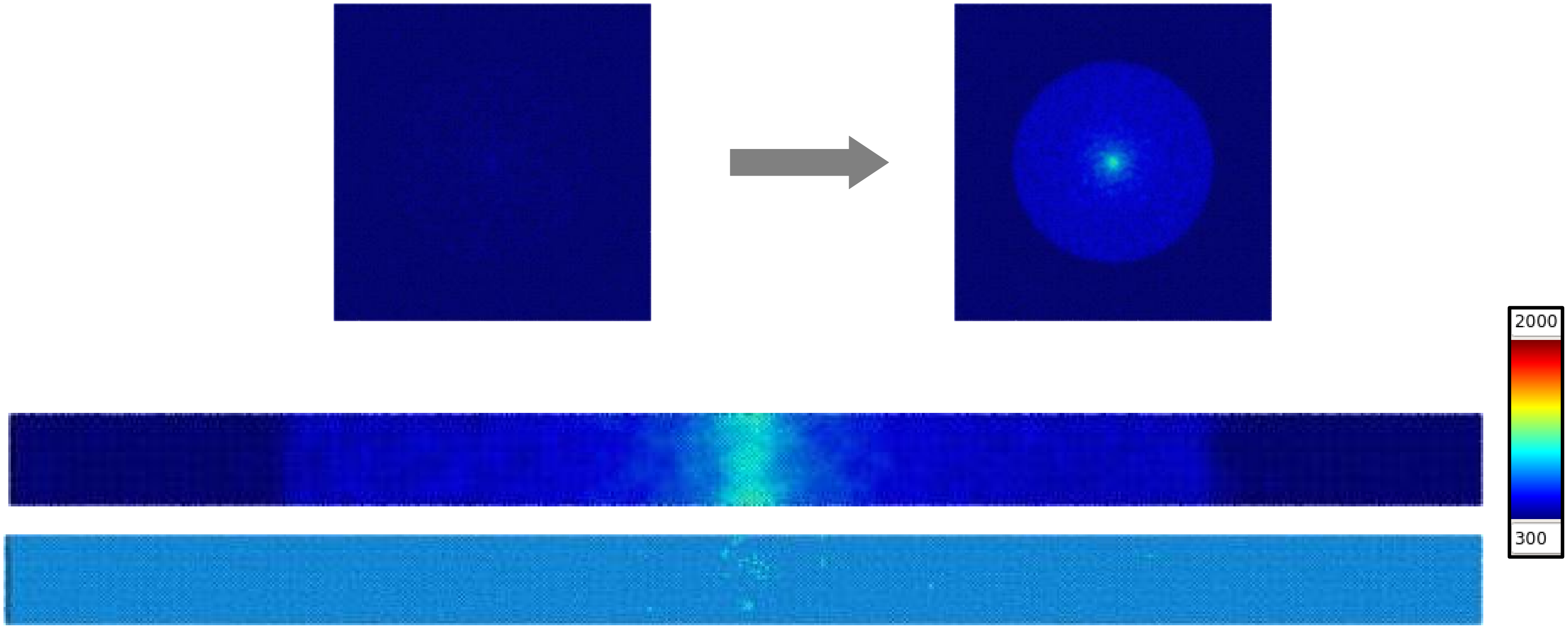


5000
4000
3000
2000
1000
0
Temperature [K]
0
2
4
6
8
10
Time [ps]



0 ps
2.5 ps
5 ps
7.5 ps

Thermal Spike, MD simulations



Conclusion

- The temperature effects on damage production during ion irradiation were presented. It can be seen that defects are almost non-existent in Si and C ion irradiation at high temperatures.

- This presentation shows a study of the role of coupled nuclear and electron energy deposition effects in SiC during ion irradiation.

- Calculation based on Thermal Spike model suggested that electronic energy deposition can affect on crystal structure evolution, even if increased temperature is below melting point.

The research leading to this result has been supported by the RADIATE project and the NCBR project “New Reactor Concepts and Safety Analyses for the Polish Nuclear Energy Program”, POWR.03.02.00-00-I005/17 (years 2018-2023).

Thank you for attention

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