Simulation of ion irradiation damage in Silicon Carbide

NATIONAL CENTRE FOR NUCLEAR RESEARCH ŚWIERK

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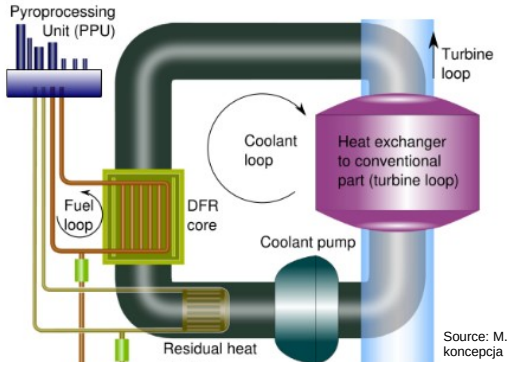
New reactor concepts and safety analyses for the Polish Nuclear Energy Program
POWR.03.02.00-00.I005/17

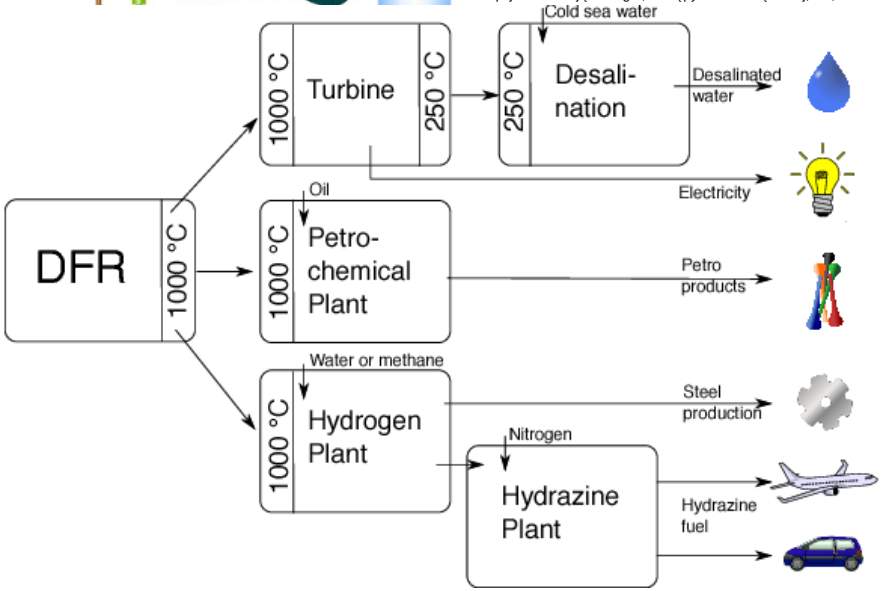
Dual Fluid Reactor

- The dual fluid reactor (DFR) is a novel concept of very high temperature nuclear reactor
- DFR design allows for an operating temperature of 1000^{o}C
- DFR needs very high temperature resistant materials that retain their mechanical properties and withstand corrosion processes under a large neutron flux
- Hard ceramics (such as **Silicon Carbide**, **Zirconium Carbide** or **Titanium Carbide**) can be a good construction material for the DFR



Dual Fluid Reactor

Source: M. P. Dąbrowski; „Reaktor Dwupłynowy jako nowa i rewolucyjna koncepcja reaktora jądrowego"; Postępy Techniki Jądrowej; z.3; 2018



Soruce: A. Huke, G. Ruprecht, D. Weißbach, K. Czerski, S. Gottlieb, A. Hussein, F. Herrmann; „Dual-fluid reactor"; Molten Salt Reactors and Thorium Energy; 2017; p. 619-633

Dual Fluid Reactor

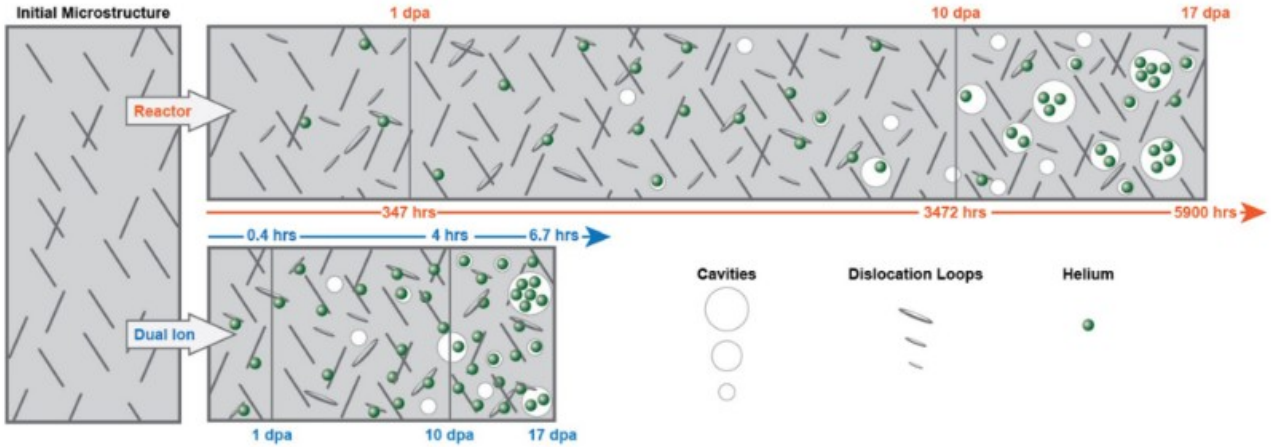
Construction Material

Irradiation Resistance

Irradiation Experiments & Simulations

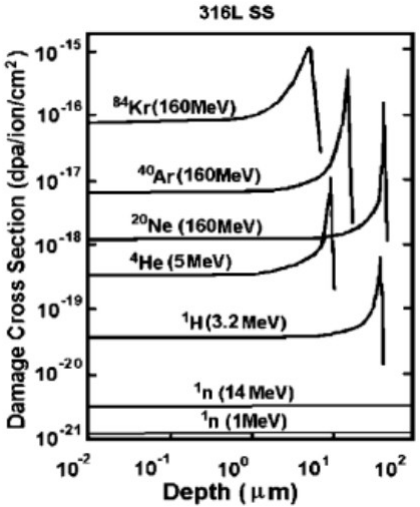
Ion vs neutron irradiation

Ion irradiation can be use as surrogate of neutron irradiation



Schematic of the time-dependent helium trapping and release behavior under reactor and ion irradiation conditions

(Source: Taller, Stephen, VanCoevering, Gerrit, Wirth, Brian D., and Was, Gary S. Predicting structural material degradation in advanced nuclear reactors with ion irradiation. United States: N. p., 2021. Web. doi:10.1038/s41598-021-82512-w.)



Comparison of damage cross sections for different ion and neuron beams

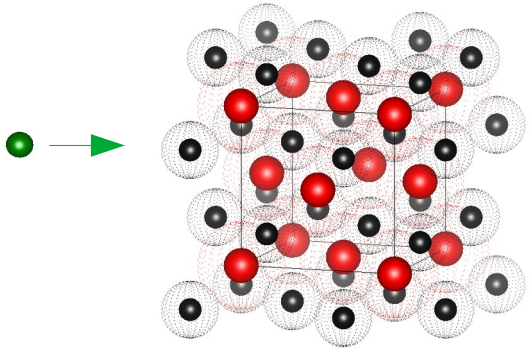
	At the first wall	DPA rate
Fission reactor (fission neutrons)	$10^{14}\frac{n}{cm^2 s}$	$< 3\frac{dps}{y}$
Fusion reactor (14MeV neutrons)	$2.0\frac{MW}{m^2}$	$20\frac{dps}{y}$
High Energy heavy ion irr.	$10^{11-13}\frac{ion\,s}{cm^2 s}$	$26\ 2600\frac{dps}{y}$

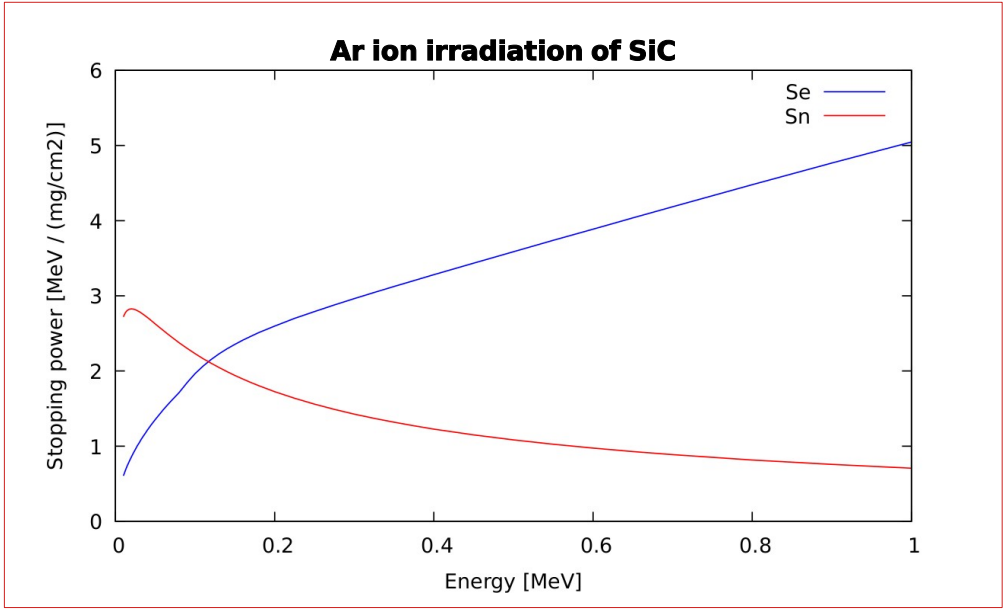
Atomic displacement rate for different radiation source

(Source: Shengyun Zhu; „Heavy Ion Irradiation Simulation of High Dose Irradiation Induced Radiation damage in Materials"; IAEA Technical Meeting on Accelerator Simulation and Theoretical Modeling of Radiation Effects; 2008; Kharkov, Ukraine)

The Stopping and Range of Ions in Matter

When **energetic ions penetrate the solid**,
it looses its energy in two way:
→ **Nuclear energy loss** due to elastic collision with atoms of the solid (dominant at low energies)
→ **Electronic energy loss** due to inelastic collisions (dominant in higher energies)





TRIM for calculating vacancy production

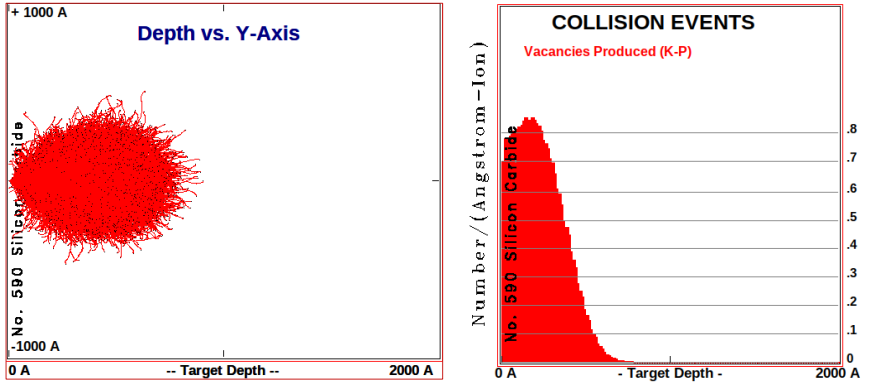
Stopping and Range of Ions in Matter (SRIM) is group of progrms that calculate interaction of ions with matter.

The core of SRIM is Transport of Ions in Matter (TRIM) program.

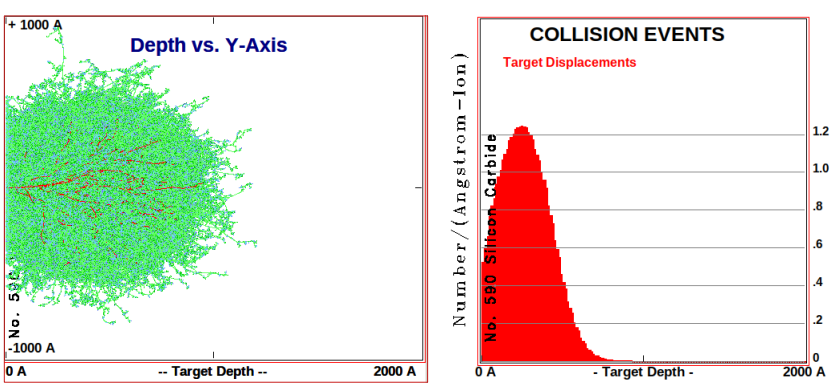
Two options of TRIM code can be use to calculate vacancy productiod during passage of ions through matter:

- **Ion Distribution and Quick Calculation Damage (Q-C)**
- **Detailed Calculation and full Damage Cascades (F-C)**

Ion Distribution and Quick Calculation Damage (Q-C)
Ion: Ar, Ion Energy: 50 keV, 50000 ions



Detailed Calculation and full Damage Cascades (F-C)
Ion: Ar, Ion Energy: 50 keV, 50000 ions



Damage energy method

The Norgett–Robinson–Torrens displacements per atom model

$$N_D = \frac{0.8 T_d}{2 E_d}$$

The damage energy

$$T_d = E_i^0 - E_i^I - E_t^I$$
$$T_d = E_i^p + E_t^p$$
$$T_d = E_t^0 - E_t^I$$
$$T_d = E_i^0 - E_i^I - E_t^I - E_i^p$$
$$T_d = E_t^p - E_i^p$$

The effective displacement energy

$$E_d^{eff} = [\sum_i \frac{S_i}{E_d^i}]^{-1}$$

S_i - the stoichiometric fraction,

E^i_d is displacement energy of the i-th atomic species

T_d - damage energy,

E_d - displacement energy,

E^0_i - incident ion energy or beam energy,

E^0_t - incident target atom energy

E^I_i - beam energy lost ionization,

E^I_t - target atom energy lost ionization,

E^p_i - beam energy lost to phonons,

E^p_t - target atom energy lost to phonons

Source:
- S. Agarwal, Y. Lin, C. Li, R.E. Stoller, S.J. Zinkle,
  On the use of SRIM for calculating vacancy production: Quick calculation and full-cascade options,
  Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms,
  Volume 503, 2021, pages 11-29, ISSN 0168-583X, https://doi.org/10.1016/j.nimb.2021.06.018
- R.E. Stoller, M.B. Toloczko, G.S. Was, A.G. Certain, S. Dwaraknath, F.A. Garner,
  On the use of SRIM for computing radiation damage exposure,
  Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms,
  Volume 310, 2013, pages 75-80, ISSN 0168-583X, https://doi.org/10.1016/j.nimb.2013.05.008.

TRIM for calculating vacancy production

Q-C vacancy calculation

Ion	1	2	3	4	5	6
Ar 10 keV	94	102	103	98	98	93
Ar 50 keV	383	418	410	408	408	390
Ar 100 keV	654	716	701	702	702	672
Ar 1 MeV	2412	2679	2623	2623	2623	2512

F-C vacancy calculation

Ion	1	2	3	4	5	6
Ar 10 keV	152	89	87	84	84	77
Ar 50 keV	549	346	333	335	335	311
Ar 100 keV	908	580	558	564	564	525
Ar 1 MeV	3273	2123	2047	2057	2057	1915

1. *Vacancy.txt*
2. $T_d = E_i^0 - E_i^I - E_t^I$
3. $T_d = E_i^p + E_t^p$
4. $T_d = E_t^0 - E_t^I$
5. $T_d = E_i^0 - E_i^I - E_t^I - E_i^p$
6. $T_d = E_t^p - E_i^p$

The displacement energies of SiC used in simulations

	Si	C
Threshold displacement energy	38 eV	19 eV
Lattice binding energy	3.25 eV	2.63 eV
Surface binding energy	4.7 eV	7.4 eV

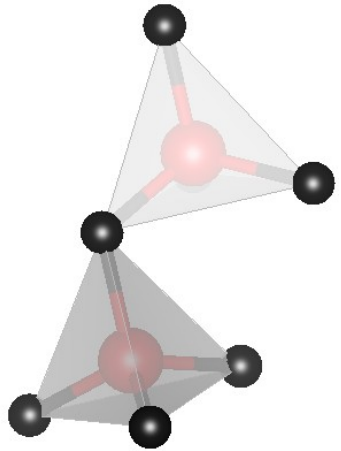
Sources: Zinkle, S. and Kinoshita, C. (1997). Defect production in ceramics. Journal of Nuclear Materials, 251:200–217. Proceedings of the International Workshop on Defect Production, Accumulation and Materials Performance in an Irradiation Environment; CHANG, J.-Y., GIL, C.-S., and LEE, W.-J. (2014). A simple method to calculate the displacement damage cross section of silicon carbide. Nuclear Engineering and Technology, 46(4):475–480;

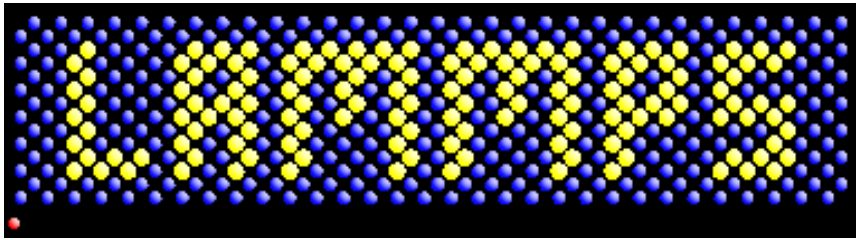
Large-scale Atomic/Molecular Massively Parallel (LAMMPS):

- is a classical molecular dynamics simulation code
- solve Newton's equation of motion

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

- consider: effect of irradiation temperature,
- effect of crystal structure
  and crystal defects
- possible study of post-irradiation relaxation
- irradiation events - primarily interact
  with atomic nuclei
- needs additional fix to simulate
  the effects of electronic excitations





Source: https://www.lammps.org/

Silicon Carbide

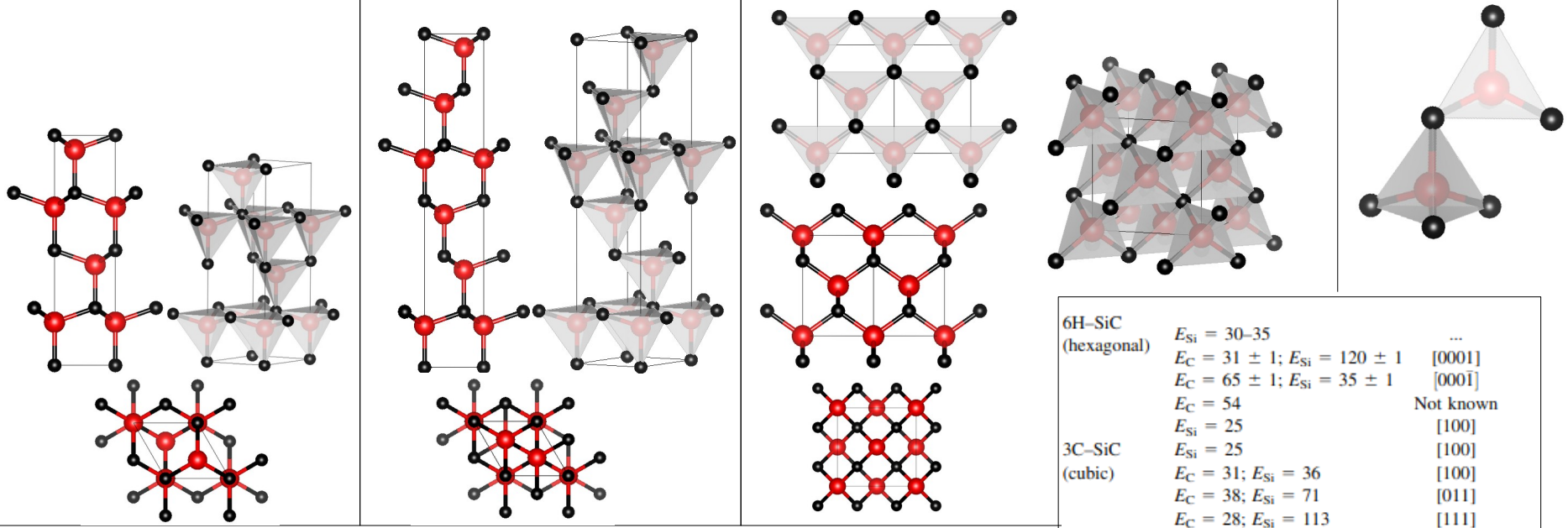
Hexagonal SiC

Cubic SiC

4H-SiC

6H-SiC

3C-SiC

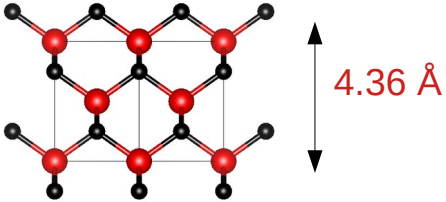


Picture generated in VESTA with data from: materialsproject.org

6H–SiC (hexagonal)	E_{Si} = 30–35	...
	$E_C = 31 \pm 1$; $E_{Si} = 120 \pm 1$	[0001]
	$E_C = 65 \pm 1$; $E_{Si} = 35 \pm 1$	[000$\bar{1}$]
	E_C = 54	Not known
	E_{Si} = 25	[100]
3C–SiC (cubic)	E_{Si} = 25	[100]
	$E_C = 31$; $E_{Si} = 36$	[100]
	$E_C = 38$; $E_{Si} = 71$	[011]
	$E_C = 28$; $E_{Si} = 113$	[111]

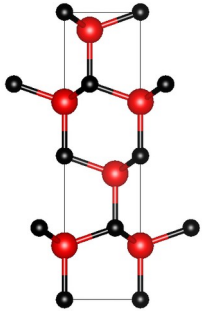
Source: D. Simeone et al.: Characterization of radiation damage in ceramics: Old challenge new issues?

Silicon Carbide



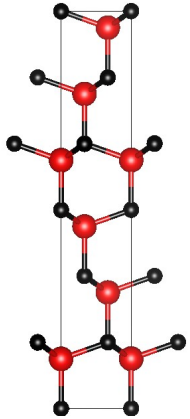
4.36 Å

3C-SiC



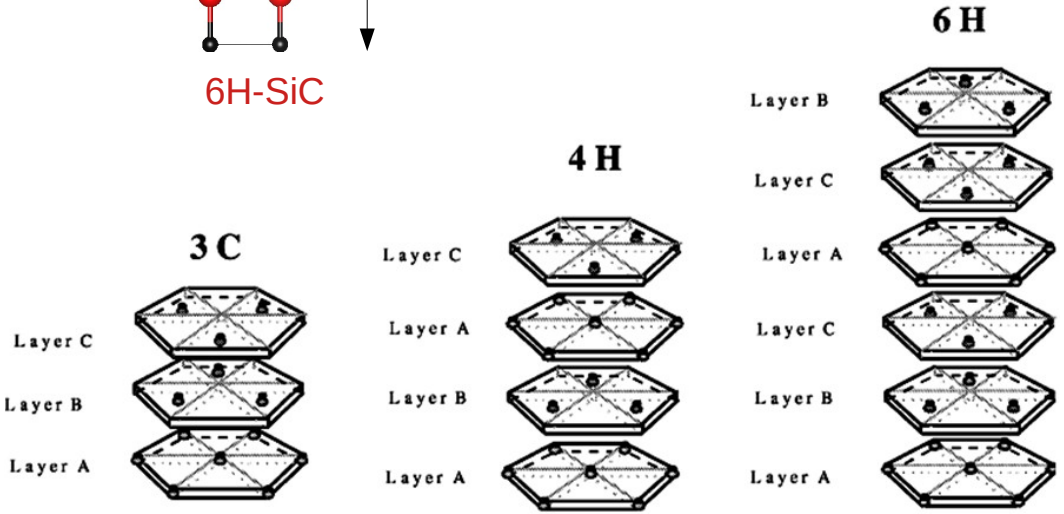
10.053 Å

4H-SiC



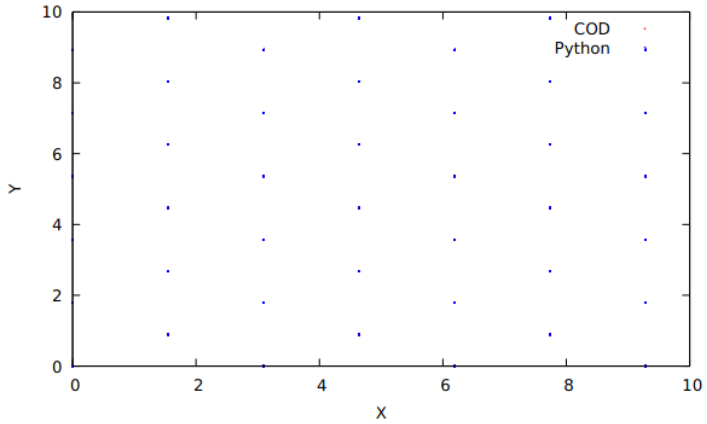
15.117 Å

6H-SiC



Source: Ching W. Y. Xu-N Y. Rulis P. Ouyang L. 2006 The Eletronic Structure and Spectroscopic properties of 3C, 2H, 4H, 6H, 15R and 21R polymorphs of SiC. Materials Science and Engineering A, 422 1-2 , (April 2006), 147 156 , 0921-5093

6H-SiC


COD
Python
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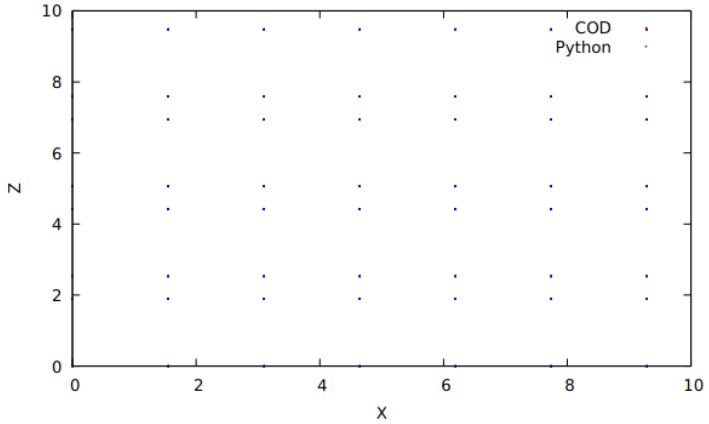
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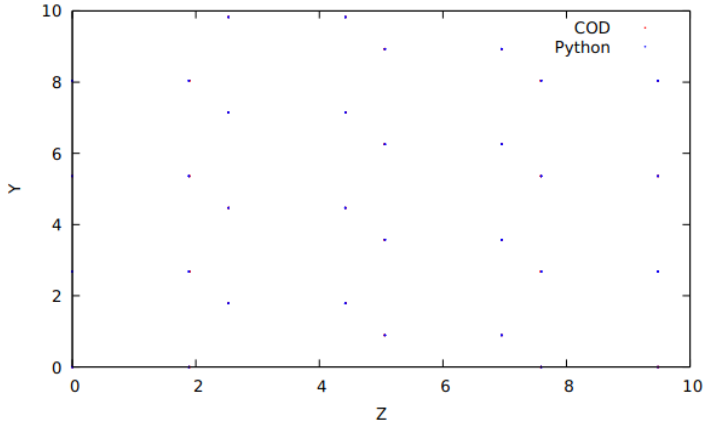
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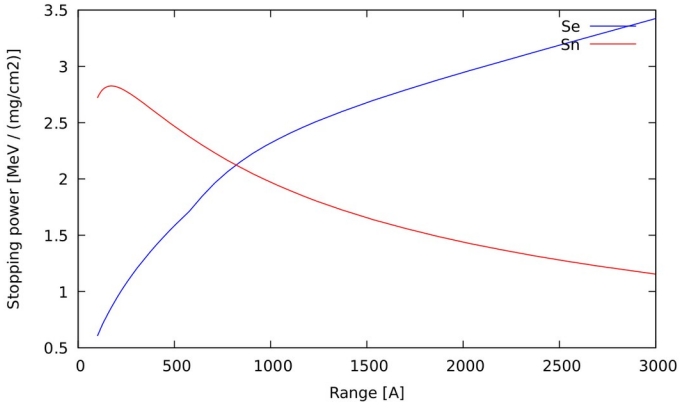
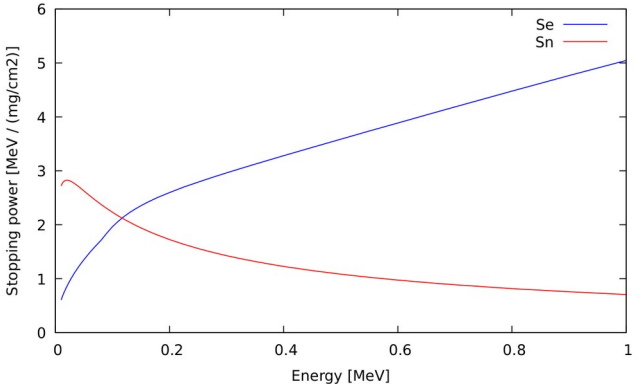
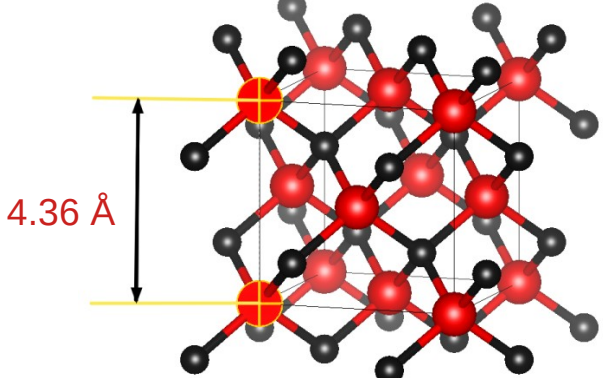
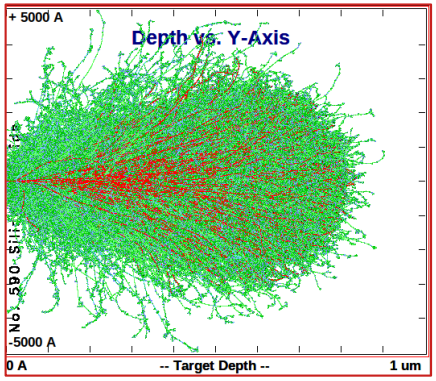
SiC sample in LAMMPS







Ion energy	S_e/S_n	Range	Range/a
50 keV	0.5	371 A	86
5 MeV	52.1	2.01 um	463
500 MeV	1938.5	122.06 um	28 070

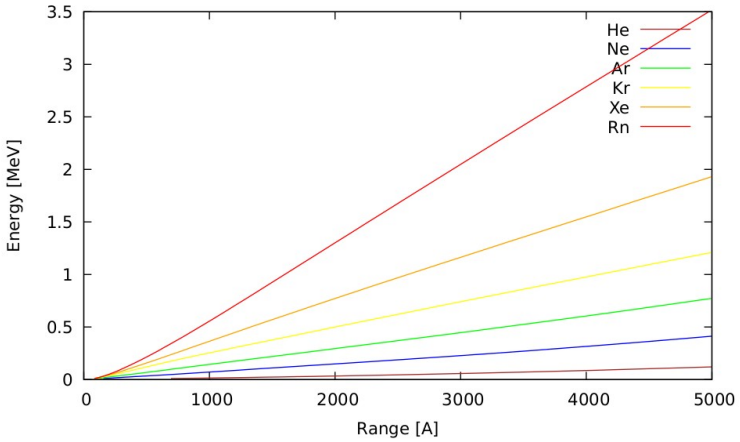


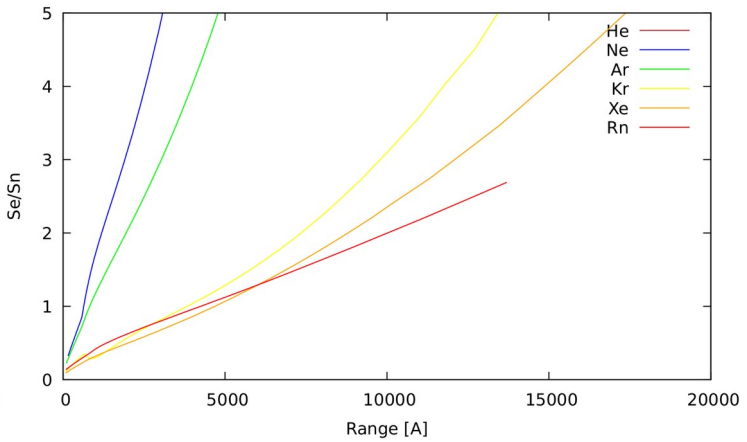
1MeV Ar in SiC

The Stopping and Range of Ions in Matter

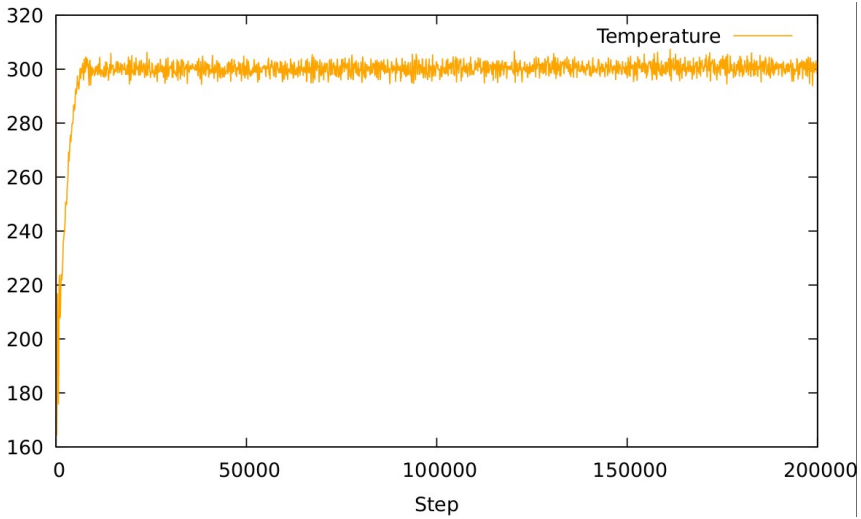
Q-C vacancy calculation

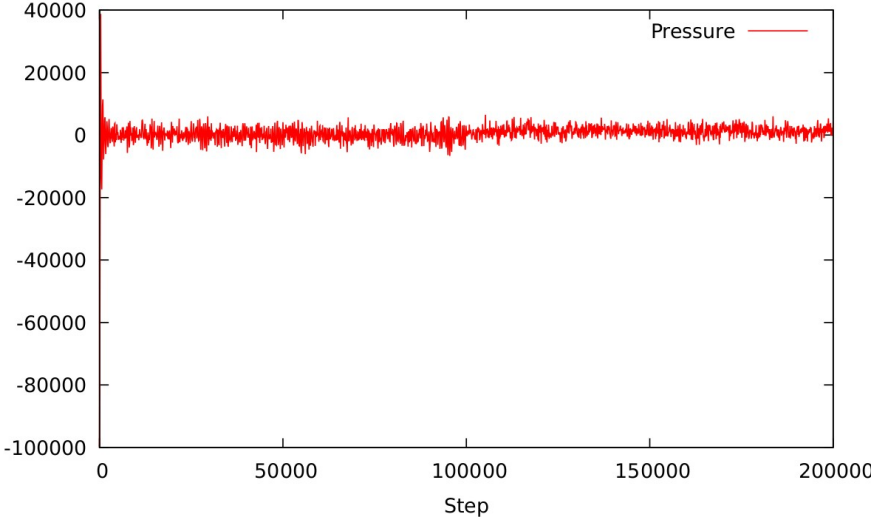
Ion	1	2	3	4	5	6
He 10 keV	31	37	41	29	30	28
Ne 10 keV	92	99	100	93	93	89
Ar 10 keV	94	102	103	98	98	93
He 50 keV	56	66	73	55	55	52
Ne 50 keV	331	361	358	348	348	333
Ar 50 keV	383	418	410	408	408	390
He 100 keV	64	75	83	62	63	59
Ne 100 keV	506	554	548	536	536	513
Ar 100 keV	654	716	701	702	702	672



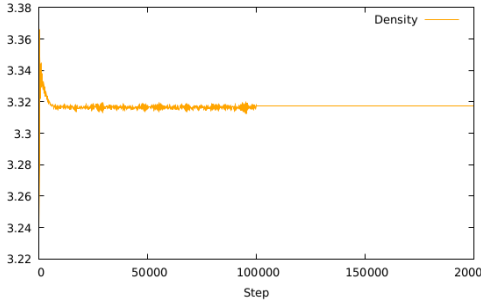


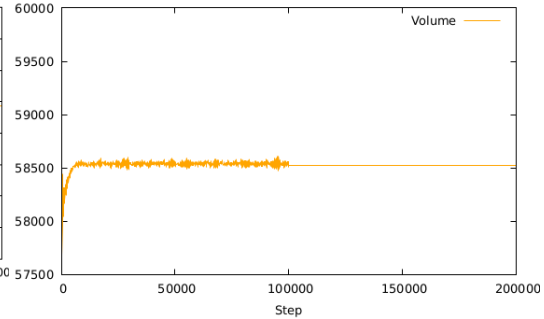
LAMMPS



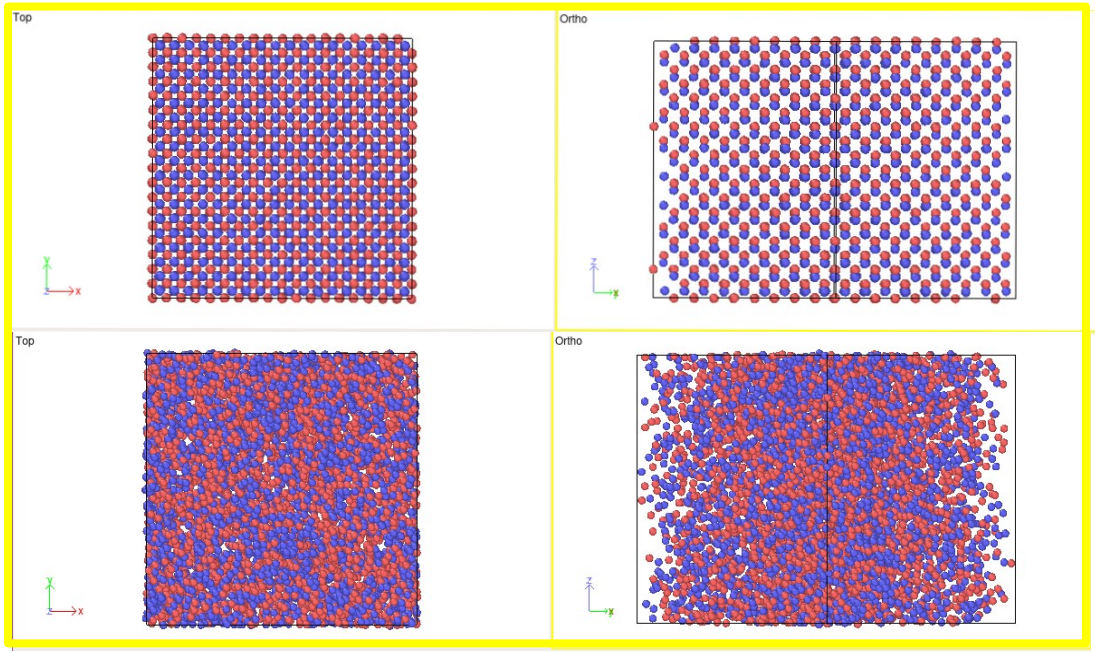


SiC sample
heated to temperature of 300 K





OVITO software is use for visualization and analysis

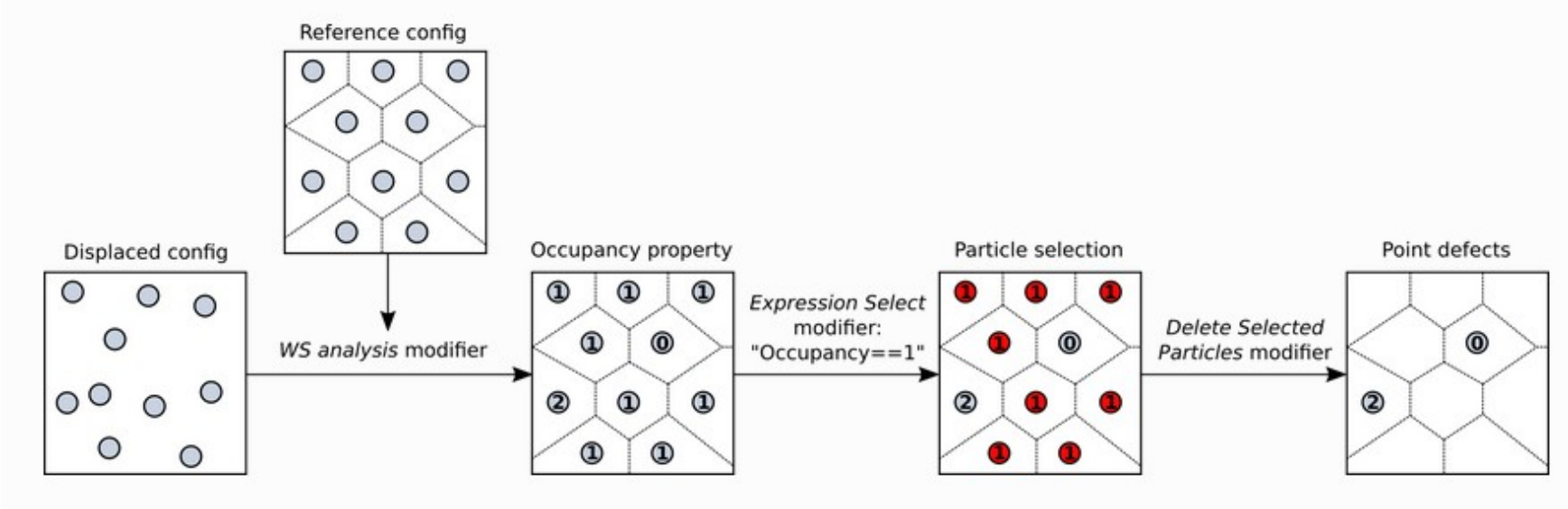


SiC sample
heated to temperature of 1 000 K

SiC sample
heated to temperature of 6 000 K

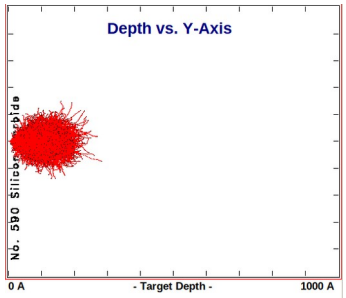
Wigner - Seitz defect analysis

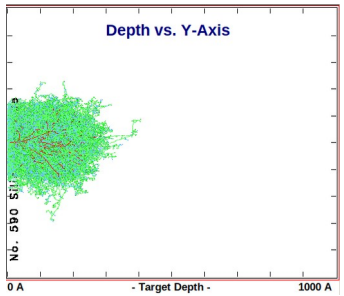
Vacancies and interstitials counting is possible due to Wigner – Seitz defect analysis in OVITO

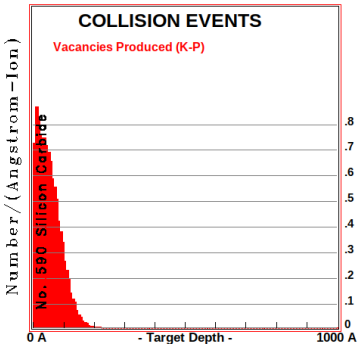


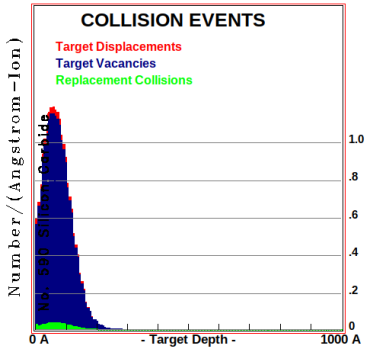
Source: https://www.ovito.org/docs/current/reference/pipelines/modifiers/wigner_seitz_analysis.html#particles-modifiers-wigner-seitz-analysis

10 keV Ar









Vacancy calculation in TRIM

Ion	1	2	3	4	5	6	
Ar 10 keV	94	102	103	98	98	93	Q-C
Ar 10 keV	152	89	87	84	84	77	F-C

Vacancy calculation in LAMMPS: 155

time: 0.5 ps

Two temperature model

- In LAMMPS it is possible to couple classical MD with a model for the transfer and diffusion of electronic energy by use two temperature model
- During heavy ion passage through matter energy is exchanged between the nuclei and electrons via electronic stopping and electron-phonon coupling mechanisms
- 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

$$C_e \rho_e \frac{\partial T_e}{\partial t} = \nabla(\kappa_e \nabla T_e) - g_p(T_e - T_a)$$

$$C_l \rho_l \frac{\partial T_l}{\partial t} = \nabla(\kappa_l \nabla T_l) + g_p(T_e - T_a)$$

$T_{e,l}(r,t)$, $C_{e,l}(r,t)$ and $K_{e,l}(r,t)$ - the temperature, the heat capacity per unit Volume, the thermal conductivity of the electronic (e) and lattice (l) subsystem, g - the electron–phonon coupling strength

Source: S.L. Daraszewicz, D.M. Duffy / Nuclear Instruments and Methods in Physics Research B 269 (2011) 1646–1649

Two temperature model

Energy transport within the electronic subsystem is solved according to the heat diffusion equation with added source terms for heat transfer between the subsystems

$$C_e \rho_e \frac{\partial T_e}{\partial t} = \nabla(\kappa_e \nabla T_e) - g_p(T_e - T_a) + g_s T'_a$$

$$g_p = \frac{3Nk_B\gamma_p}{\triangle V m_1}$$

$$g_s = \frac{3N'k_B\gamma_s}{\triangle V m_1}$$

T_e, C_e, and K_e – the electronic temperature, the electronic heat capacity per unit Volume, the electronic thermal conductivity, T_e - the lattice temperature, g_p - the coupling constant for the electron-ion interaction, g_s - the electron stopping coupling parameter,

N is the number of atoms in a cell of volume V, N' is the number of atoms with $v > v_0$, k_B represents the Boltzmann constant

TTM model

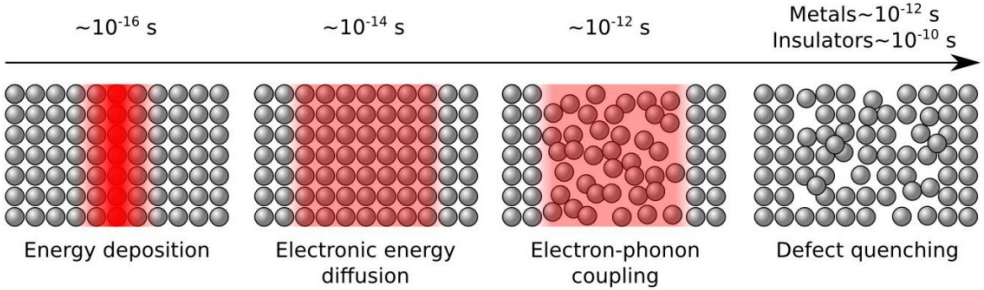
$$m_i \frac{\partial \mathbf{v_e}}{\partial t} = \mathbf{F_i}(t)$$

$$m_i \frac{\partial \mathbf{v_e}}{\partial t} = \mathbf{F_i}(t) - \gamma_i \mathbf{v_i} + \mathbf{F'_i}(t)$$

Langevin thermostat

$$m_i \frac{\partial \mathbf{v_e}}{\partial t} = \mathbf{F_i}(t) - \gamma_i \mathbf{v_i} + \mathbf{F'_i}(t)$$

- $\mathbf{F_i}(t)$: conservative force
- $\gamma_i \mathbf{v_i}$: energy loss
- $\mathbf{F'_i}(t)$: energy loss or gain



Source: https://discovery.ucl.ac.uk/id/eprint/10044834/1/Review_2T_MD_final.pdf

Electron stopping effect

$$\gamma_i = \gamma_p + \gamma_s$$

- γ_p: friction due to electron – atom interaction
- γ_s: friction due to electron stopping

Conclusion

- In this work, I have examined TRIM vacancy production different approaches:
  Quick Calculation and Full Cascades
  using the vacancy.txt and damage energy method

- Results from TRIM have been compered to vacancy calculated with use LAMMPS code
  The most similar to molecular dynamic result is
  Full Cascades with using the vacancy.txt result

- It is important to use alsso model that include electronic stopping power and electron – phonon coupling factor

Thank you for attention

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Fundusze Europejskie Wiedza Edukacja Rozwój

Rzeczpospolita Polska

Unia Europejska Europejski Fundusz Społeczny

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