Atomistic simulation of ion-beam-induced defect formation

related publications (since 2001):

Posselt, M.,
Improving the understanding of ion-beam-induced defect formation and evolution by atomistic computer simulations,
Mat. Res. Soc. Symp. Proc. 647 (2001) O2.1.1

combined simulation method

ballistic processes
energy: > 100 eV, duration: < 100 fs

BCA simulations

fast relaxation processes
energy: 1...100 eV, duration: 100 fs ...100 ps

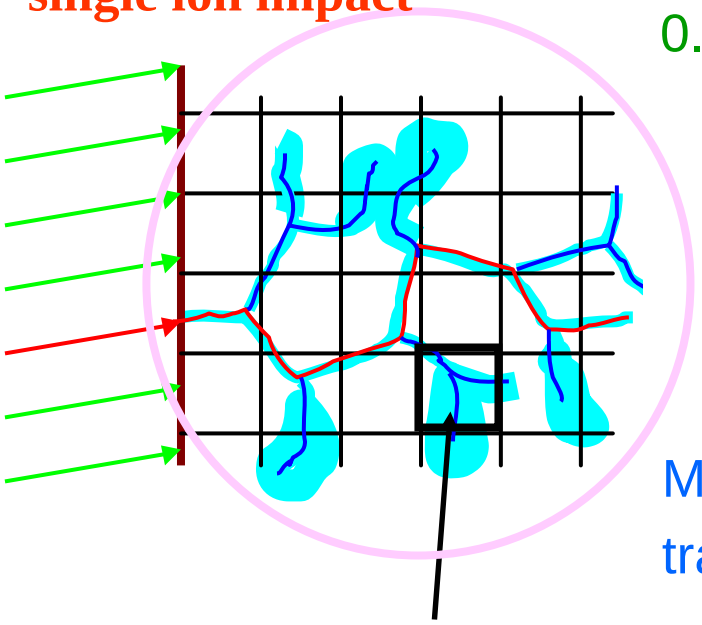
Molecular Dynamics (MD)

repulsive *and* attractive interaction between all atoms (classical potential),
semiempirical model for the ***electronic energy loss*** *of fast particles*

→defect types and morphology

top-down approach

single ion impact



cubic registration cells:
e.g. $10a_0 x 10a_0 x 10a_0$
a_0: lattice constant

BCA simulations of the **whole collision cascade** of a single ion for energy transfers > 100 eV: 0...100 fs

↓

interface

↓

MD simulation of processes starting with energy transfers < 100 eV, consideration of a part of the collision cascade in cubic **registration cells**; 100 fs ... some 100 ps

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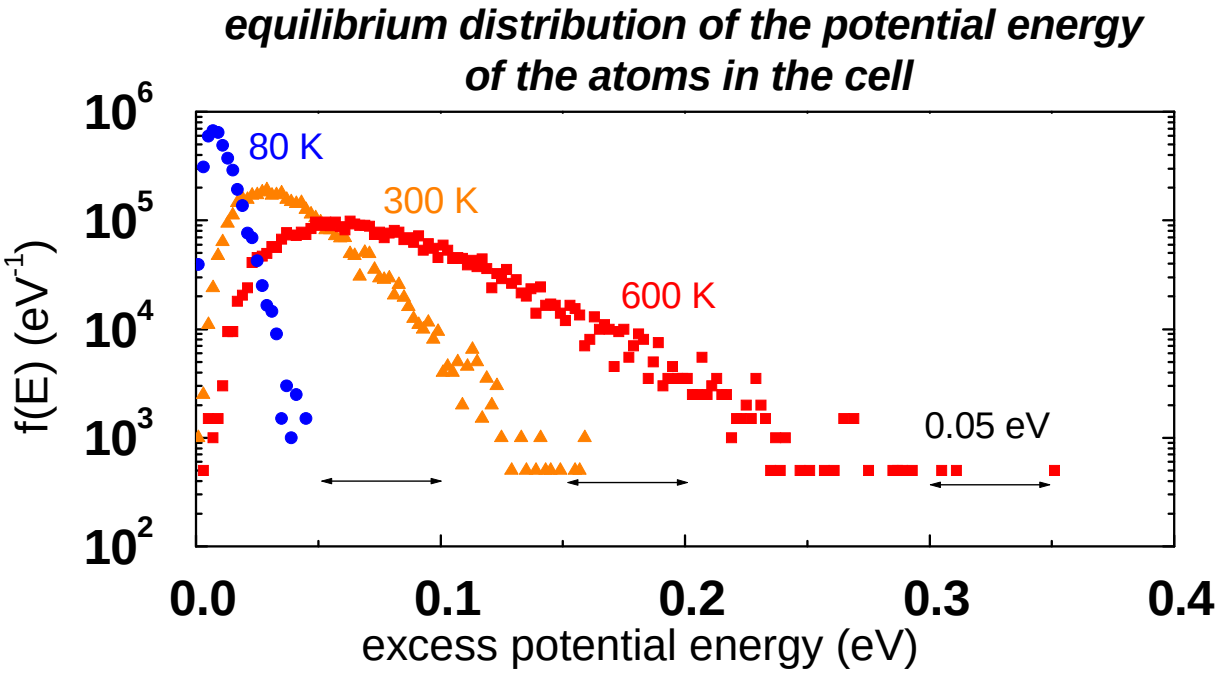
defect analysis (1)

identification of ***disordered atoms***

atoms the potential energy of which is at least

0.1 eV (T = 80 K) *0.2 eV (T = 300 K)* *0.35 eV (T = 600 K)*

above the ground state value



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defect analysis (2)

identification of **V, I**

Wigner-Seitz cell analysis using the ideal lattice as reference

*WS cell without any atoms: **V***

*each additional atom in WS cell: **I***

defect analysis (3)

visualization of **atomic defect structures**

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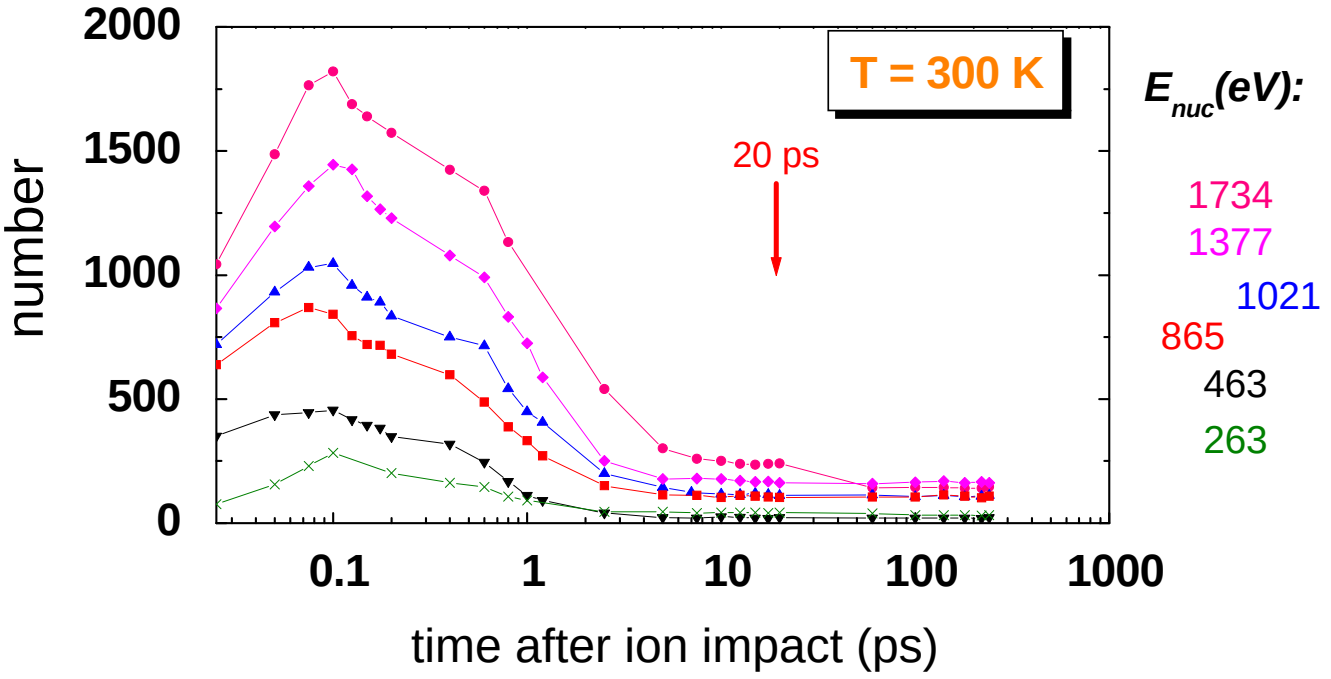
temporal evolution of the number of disordered atoms in a registration cell depends on the nuclear energy deposition E_{nuc} into the cell



fast relaxation processes are finished after 5 - 20 ps

formation of a (meta)stable defect configuration

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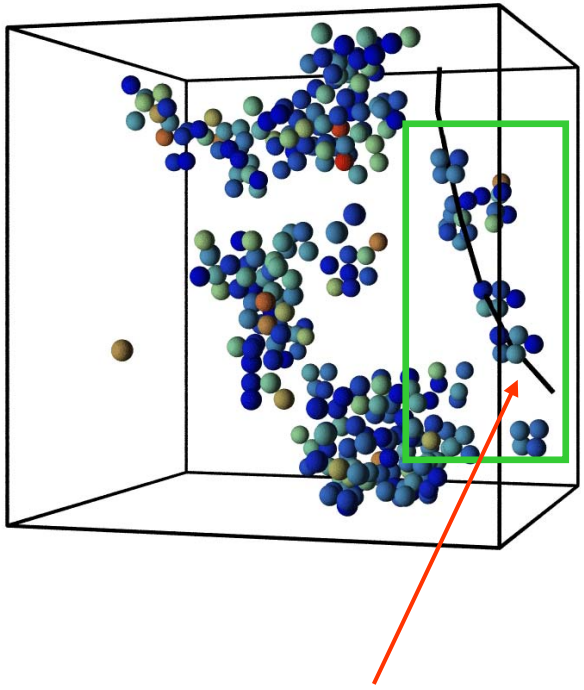
T = 300 K

E_{nuc} ~ 2400 eV

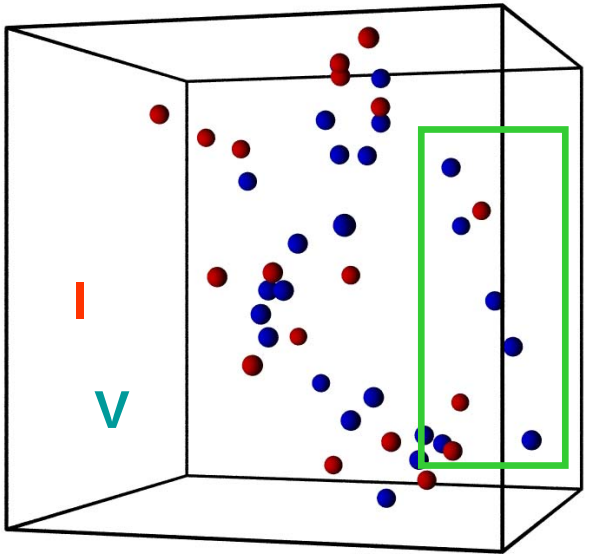
20 ps

disordered atoms



ion trajectory

V, I



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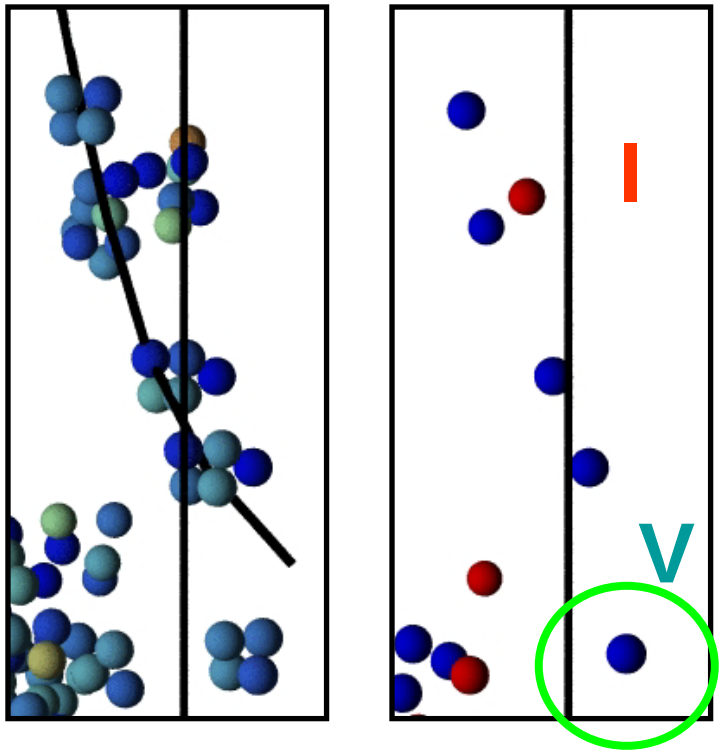
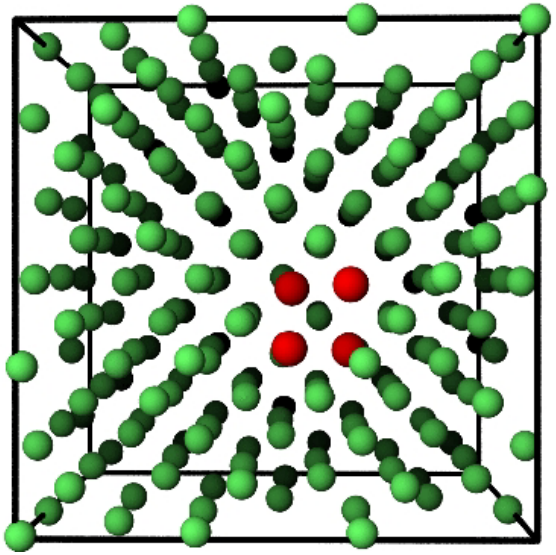
disordered atoms V,I



vacancy



(100)

T = 300 K

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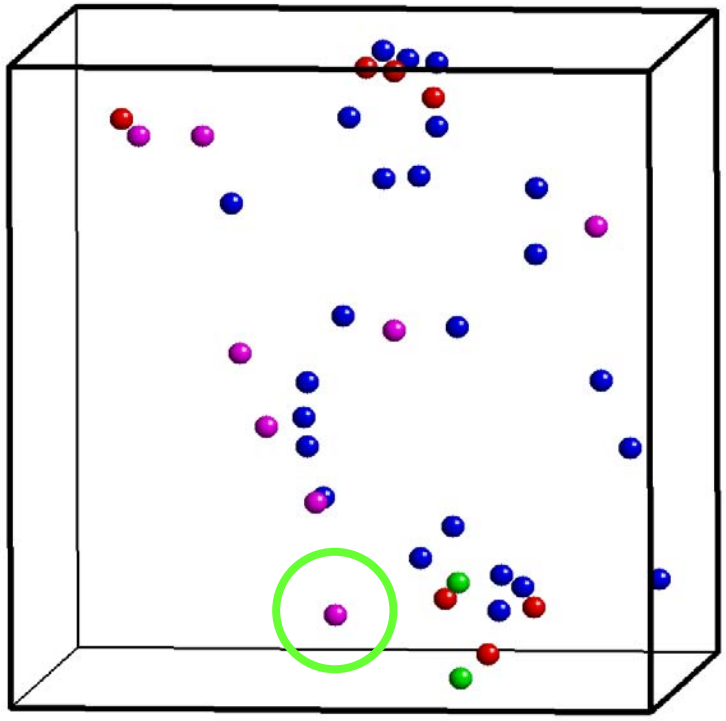
interstitial configurations



<110> dumbbells

<100> dumbbells

other structures

T = 300 K

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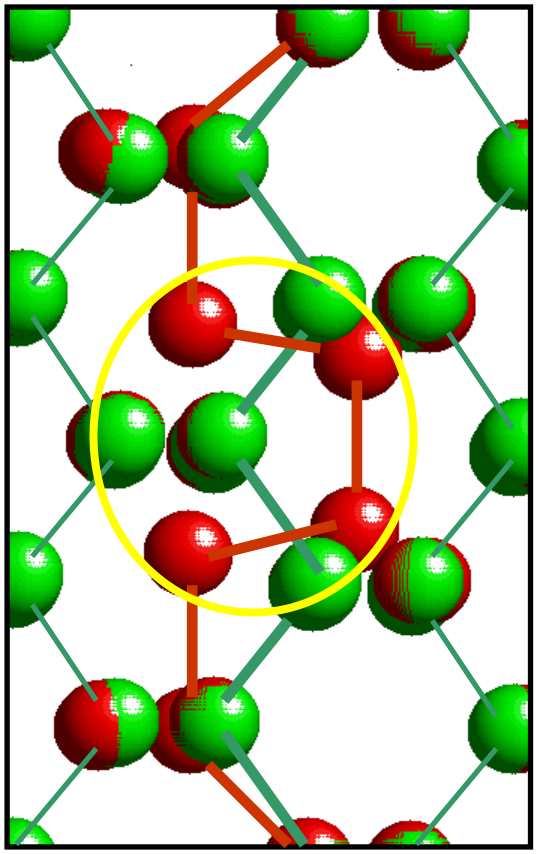
extended

<110> dumbbell



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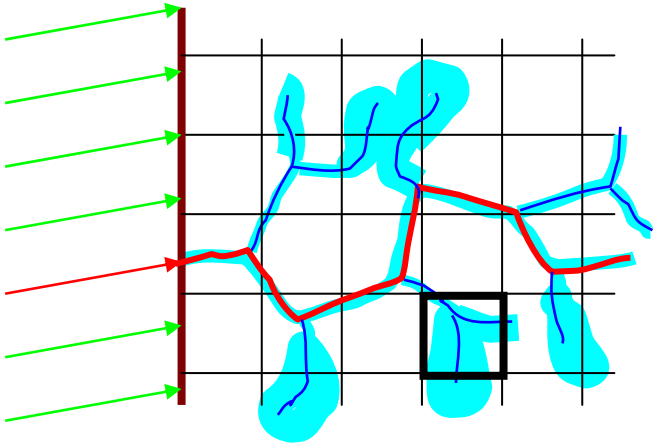
bottom-up approach

single ion impact



MD results for different values nuclear energy deposition in *a* cell

BCA: statistics of nuclear energy deposition in *all* cells

total number of certain defects per incident ion

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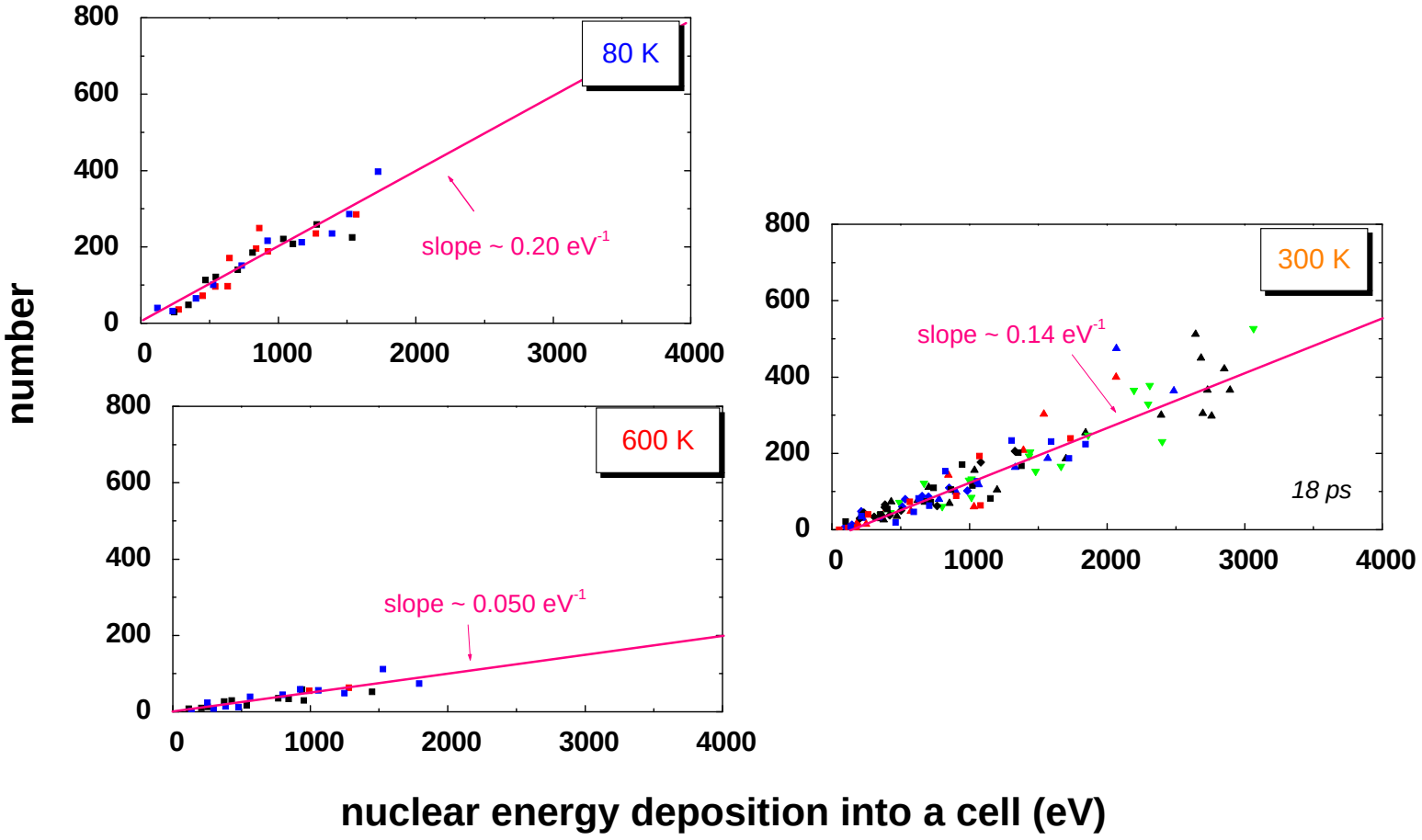
MD

number of disordered atoms



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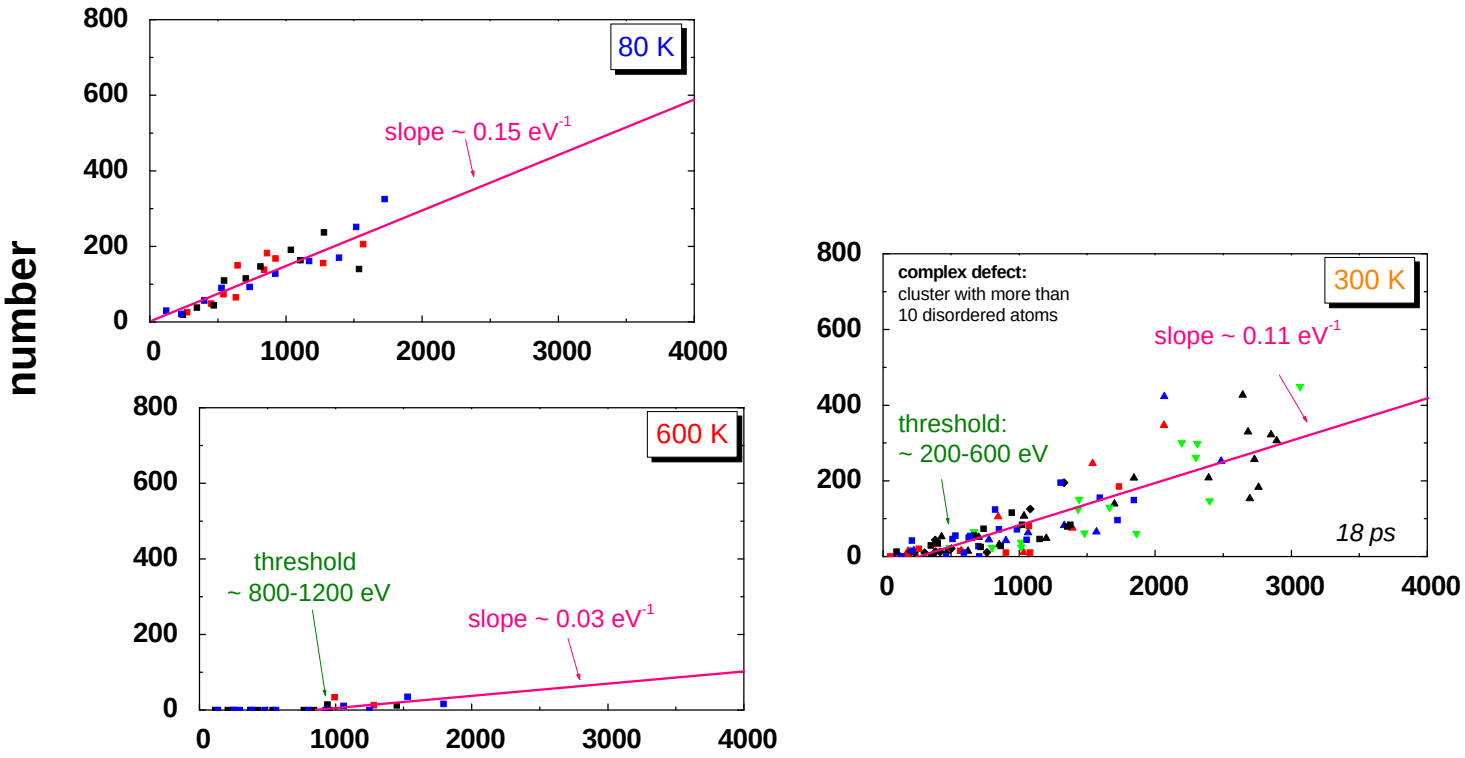
MD

number of disordered atoms in complex defects (clusters with more than 10 disordered atoms)



nuclear energy deposition into a cell (eV)

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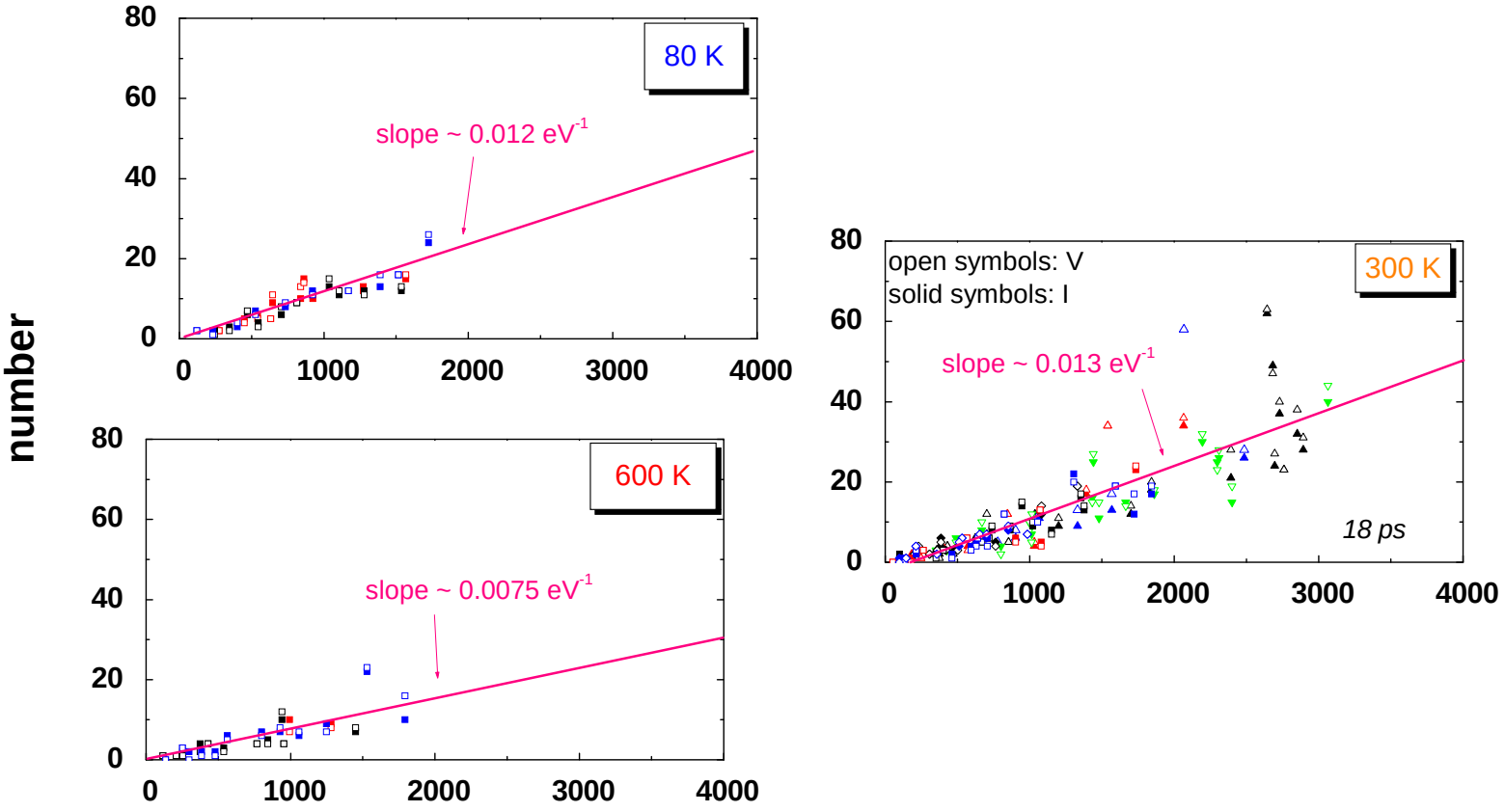
MD

total number of V and I



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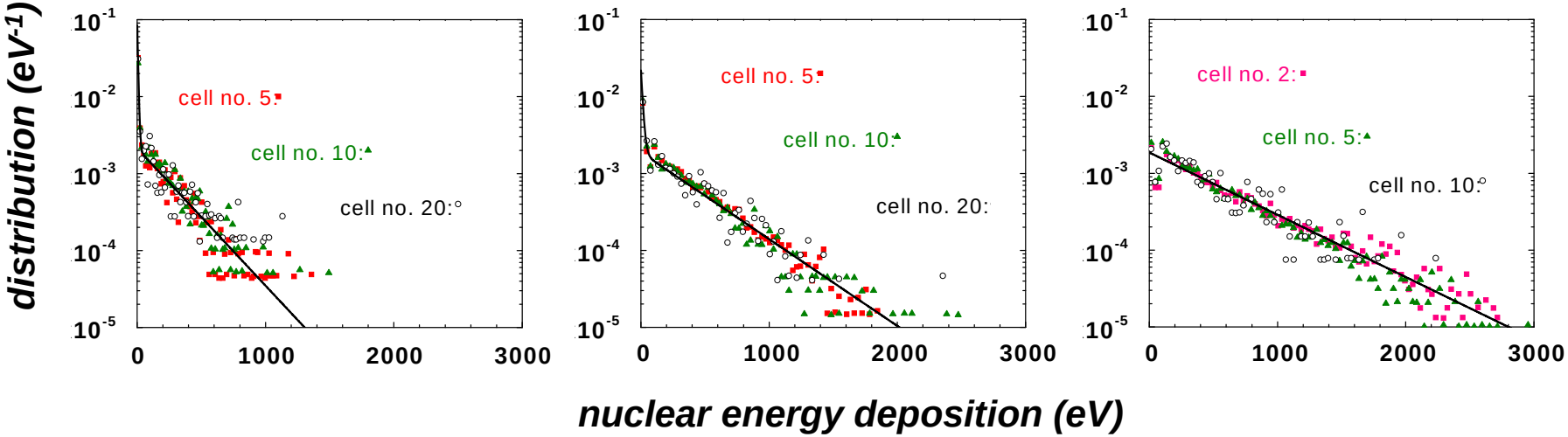
BCA

normalized distribution of nuclear energy deposition

B^+ (15 keV),
7^0 tilt, 0^0 rotation

P^+ (30 keV),
7^0 tilt, 0^0 rotation

As^+ (15 keV),
6^0 tilt, 0^0 rotation



nearly independent of the *depth* of the registration cells and the *implantation energy*

important characteristic for each ion species

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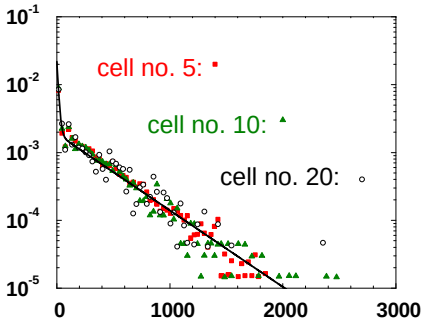
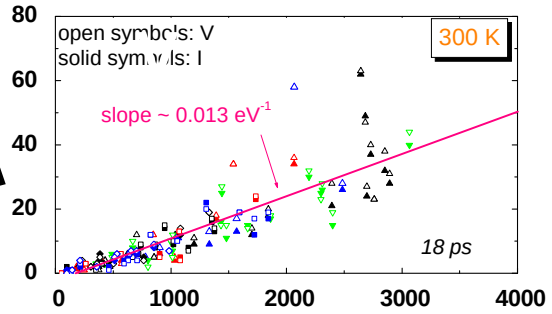
combination of BCA and MD results:

$$\sum_i \int c_i * dE_{nuc}$$

e.g. depth profile of V

(i: registration cell at certain depth)





E_{nuc}: nuclear energy deposition (eV)

e.g. total number of V formed per incident ion

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18 ps after ion impact, T = 300 K

→ **total number of defects per incident ion**

	15 keV B^+	5 keV P^+	10 keV P^+	20 keV P^+	30 keV P^+	15 keV As^+
nuclear energy deposition (eV)	3200	2000	3600	6100	8200	6700
disordered atoms total	540	293	525	902	1244	1062
in complex defects	114	87	172	299	426	464
in amorphous pockets	59	52	108	189	272	327
V or I total	50	27	49	84	115	99
isolated I (crit. II)	17	9	17	29	39	34
isolated V (crit. II)	7	4	7	12	16	13
excess of isolated I	10	5	10	17	23	21

total number of defects

divided by the total nuclear energy deposition per ion (unit: eV^{-1})

	15 keV B^+	5, 10, 20, 30 keV P^+	15 keV As^+
disordered atoms total	0.17	0.15	0.16
in complex defects	***0.036***	***0.048***	***0.069***
in amorphous pockets	***0.018***	***0.030***	***0.049***
V or I total	0.016	0.014	0.015

T = 300 K

ballistic displacements: ~ 0.025

characteristic damage morphology for each ion species

not only isolated V and I are formed