Atomistic simulation of ion implantation

Forschungszentrum Dresden Rossendorf

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M. Posselt,
Institute of Ion Beam Physics
and Materials Research

related publications (since 2001):

Zolnai, Z.; Ster, A.; Khanh, N. Q.; Battistig, G.; Lohner, T.; Gyulai, J.; Kotai, E.; Posselt, M.,
Damage accumulation in nitrogen implanted 6H SiC: Dependence on the direction of ion incidence and on the ion fluence,
J. Appl. Phys. 101 (2007) 023502

Romanek, J.; Grambole, D.; Herrmann, F.; Voelskow, M.; Posselt, M.; Skorupa, W.; Zuk, J.,
Ion implantation-induced damage depth profile determination in SiC by means of RBS/C and bevelling technique,
Nucl. Instr. Meth. B 251 (2006) 148

Posselt, M.; Bischoff, L.; Grambole, D.; Herrmann, F.,
Competition between damage buildup and dynamic annealing in ion implantation into Ge,
Appl. Phys. Lett. 89 (2006) 151918

Posselt, M., Mäder, M., Lebedev, A., Grötzschel, R.,
Multiple implantations into Si: influence of the implantation sequence on ion range profiles,
Appl. Phys. Lett. 87 (2005) 043109

Zolnai, Z., Ster, A., Khánh, N. Q., Kótai, E., Posselt, M., Battistig, G., Lohner, T., Gyulai, J.,
Ion beam analysis and computer simulation of damage accumulation in nitrogen implanted 6H-SiC: Effects of channeling,
Materials Science Forum 483-485 (2005) 637

Posselt, M., Bischoff, L., Teichert, J., Ster, A.,
Influence of dynamic annealing on the shape of channeling implantation profiles in Si and SiC,
J. Appl. Phys. 93 (2003) 1004

Posselt, M., Mäder, M., Grötzschel, R., Behar, M.,
Competing influence of damage buildup and lattice vibrations on the shape of ion range profiles in Si,
Appl. Phys. Lett. 83 (2003) 545

Guo B. N., Variam N., Jeong U., Mehta S., Posselt M., Lebedev, A.,
Channeling doping profiles studies for small incident angle implantation into silicon wafers,
AIP Conference Proceedings 680 (2003) 658

Kögler, R., Peeva, A., Lebedev, A., Posselt, M., Skorupa, W., Özelt, G., Hutter, H., Behar, M.,
Cu gettering in ion implanted and annealed silicon in regions before and beyond the main projected ion range,
J. Appl. Phys. 94 (2003) 3834

Bracht, H., Fage Pedersen, J., Zangenberg, N., Nylandsted Larsen, A., Haller, E. E., Lulli, G., Posselt, M.,
Radiation enhanced silicon self-diffusion and the silicon vacancy at high temperatures,
Phys. Rev. Lett. 91 (2003) 245502

Posselt, M., Bischoff, L., Teichert, J., Ster, A.,
Dose rate and temperature dependence of ion-beam-induced defect evolution in Si and SiC
Mat. Res. Soc. Symp. Proc. 719 (2002) F11.2

Zolnai, Z., Khánh, N. Q., Szilágyi, E., Kótai, E., Ster, A., Posselt, M., Lohner, T., Gyulai, J.,
Investigation of ion implantation induced damage in the carbon and silicon sublattices of 6H-SiC
Diamond and Related Materials 11 (2002) 1239-1242

Posselt, M., Bischoff, L., Teichert, J.,
Influence of dose rate and temperature on ion-beam-induced defect evolution in Si investigated by channeling implantation at different doses,
Appl. Phys. Lett. 79 (2001) 1444

Posselt, M., Teichert, J., Bischoff, L., Hausmann, S.,
Dose rate and temperature dependence of Ge range profiles in Si obtained by channeling implantation,
Nucl. Instr. Meth. B 178 (2001) 170

processes: energy and time scales

ballistic processes

energy: > 100 eV, duration: < 100 fs

series of consecutive binary collisions of the moving projectile with the nearest target atom (lattice structure)

repulsive interaction between the projectile and the target atom (screened Coulomb potential)

semiempirical model for the ***electronic energy loss*** *of fast particles*

Debye (-Einstein) model for ***lattice vibrations***

phenomenological models for ***damage buildup and dynamic annealing***

computer simulations based on the binary collision approximation (BCA), ***Crystal-TRIM code***

→range distribution of the implanted ions

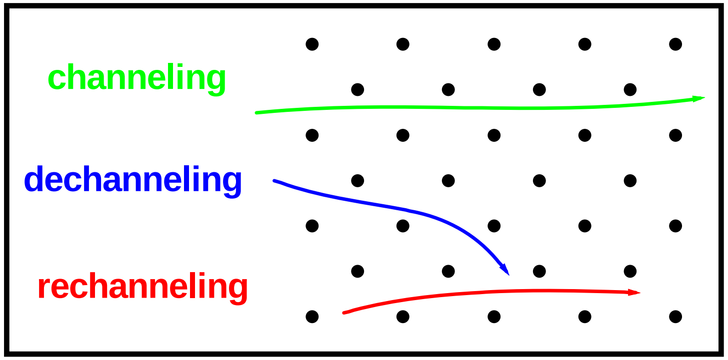
→ distribution of atomic displacements

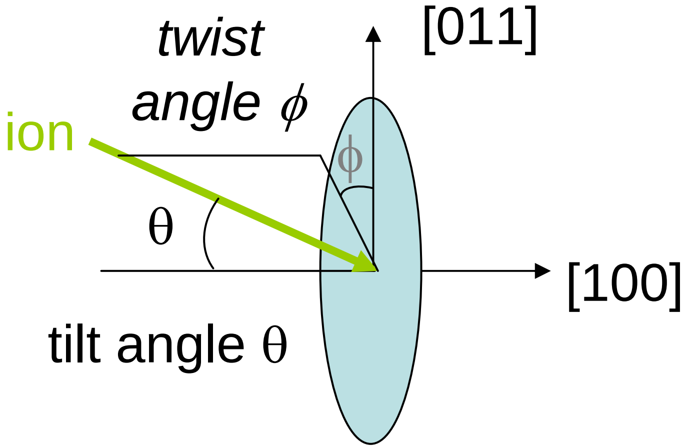
examples

low doses: example I

influence of the direction of ion incidence

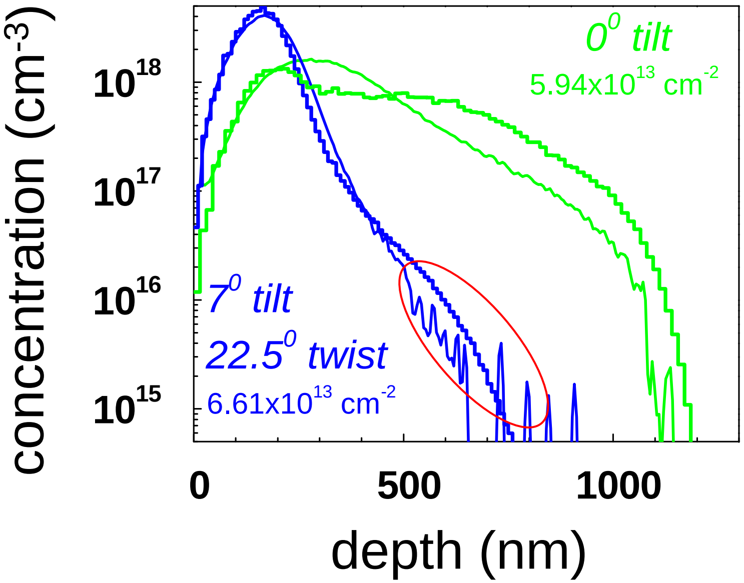
channeling effects





simulation results (histograms) vs. exp. (SIMS) data (lines):

140 keV P^+ into (100) Si



low doses: example II

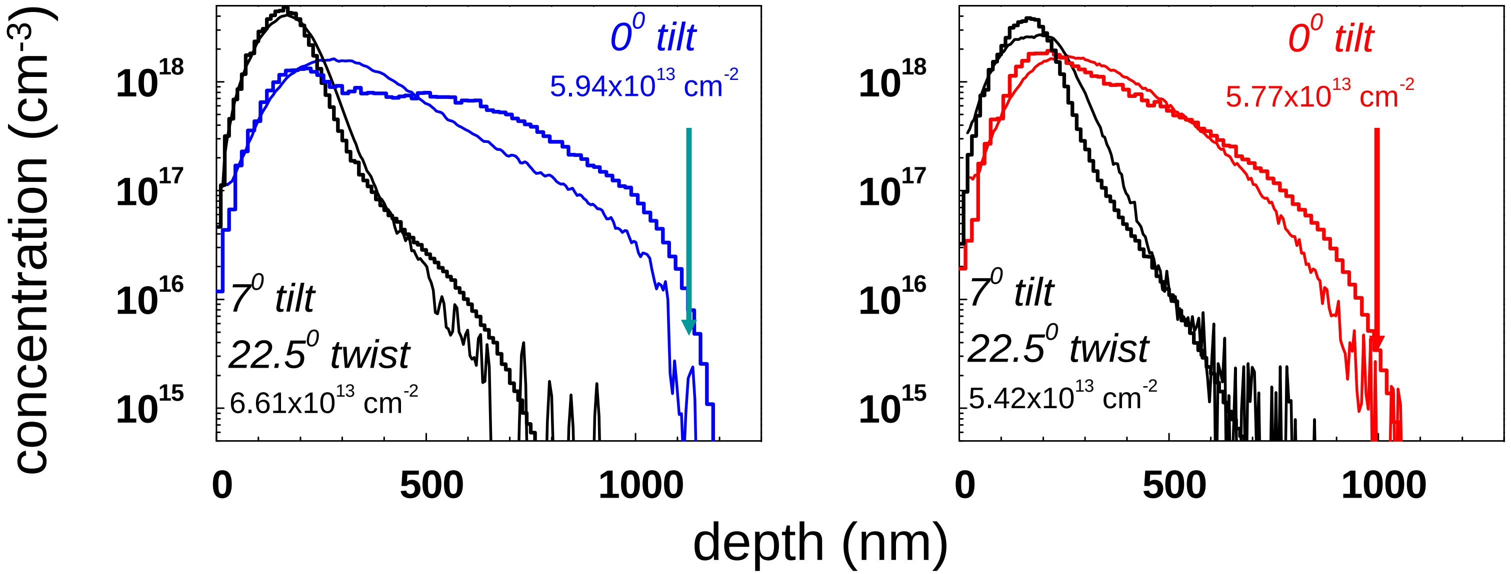
influence of the target temperature

thermal vibration of lattice atoms cause dechanneling

simulation results vs. exp. data:

140 keV P^+ into (100) Si

RT **350 ^{0}C**



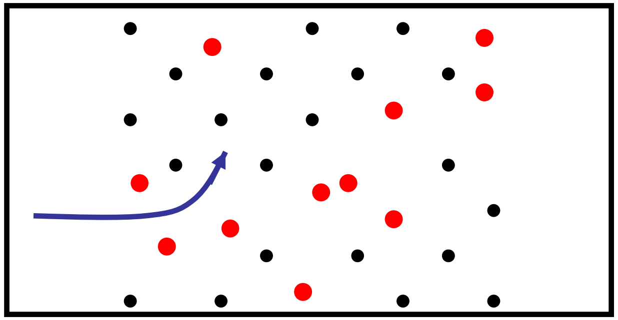
high doses: example I

dose dependence of the profile shape

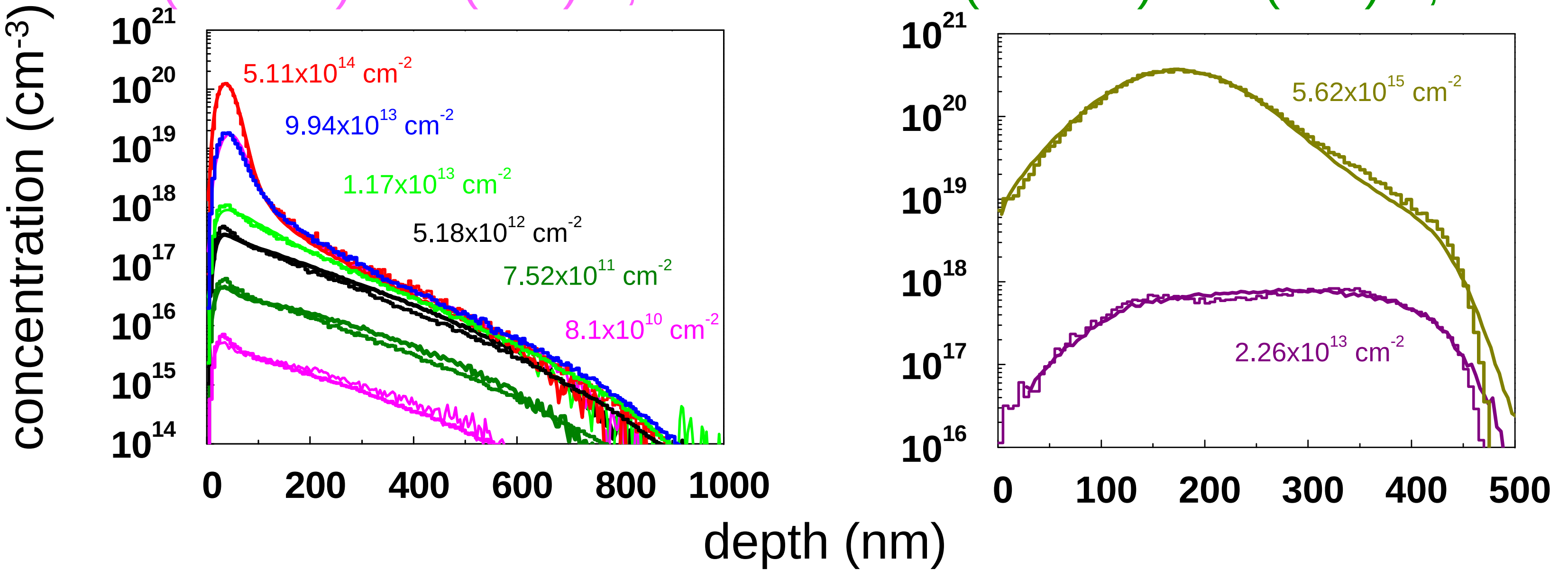
enhanced dechanneling

due to **damage buildup**

phenomenological model



simulation results vs. exp. data:



As^{+}(50 keV) into (100)Si, **0^{0} tilt**

B^{+}(35 keV) into (100)Si, **0^{0} tilt**

high doses: example II

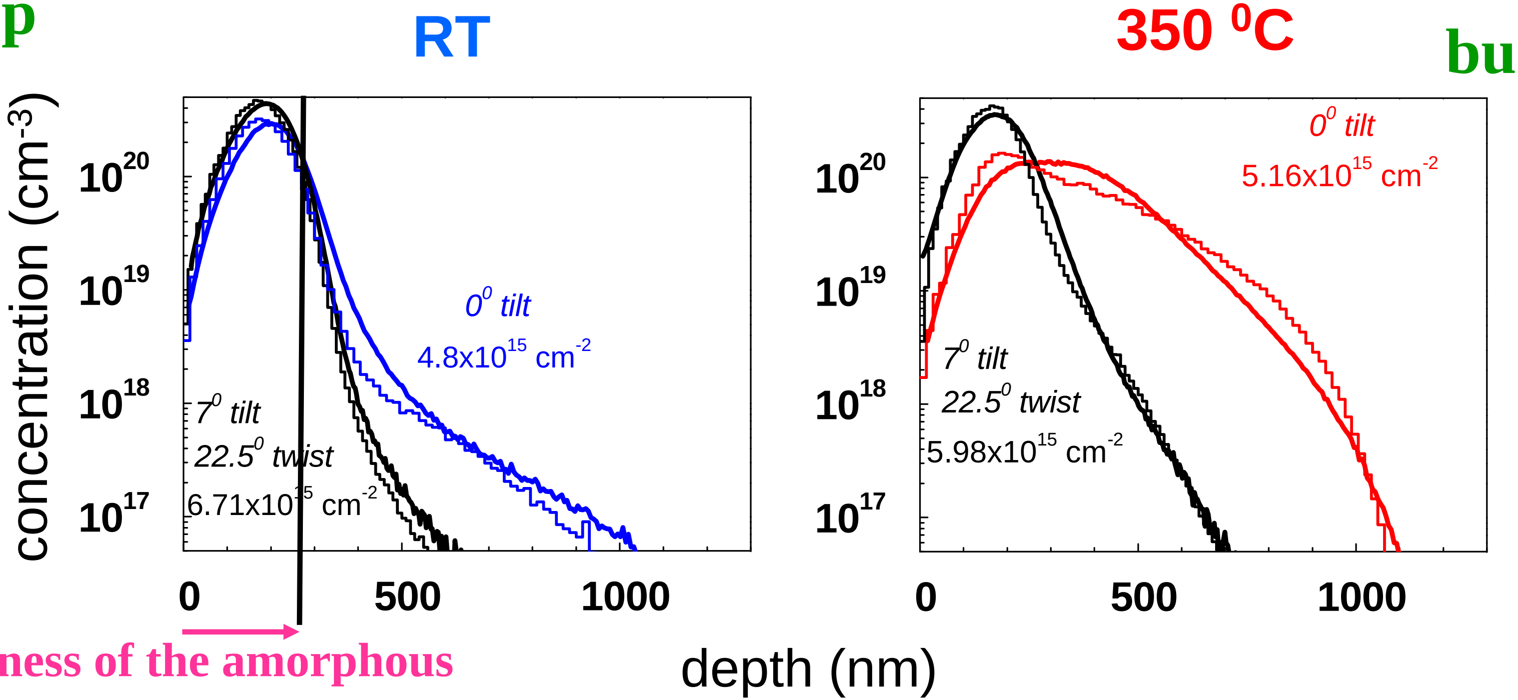
temperature dependence

damage buildup

simulation results vs. exp. data:

140 keV P^+ into (100) Si

***no* damage buildup**



thickness of the amorphous layer formed:
RBS/C: 280 nm,
Crystal-TRIM: 278 nm

high doses: example III

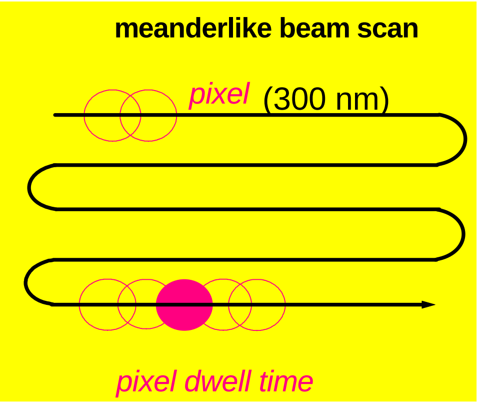
influence of dose rate and target temperature

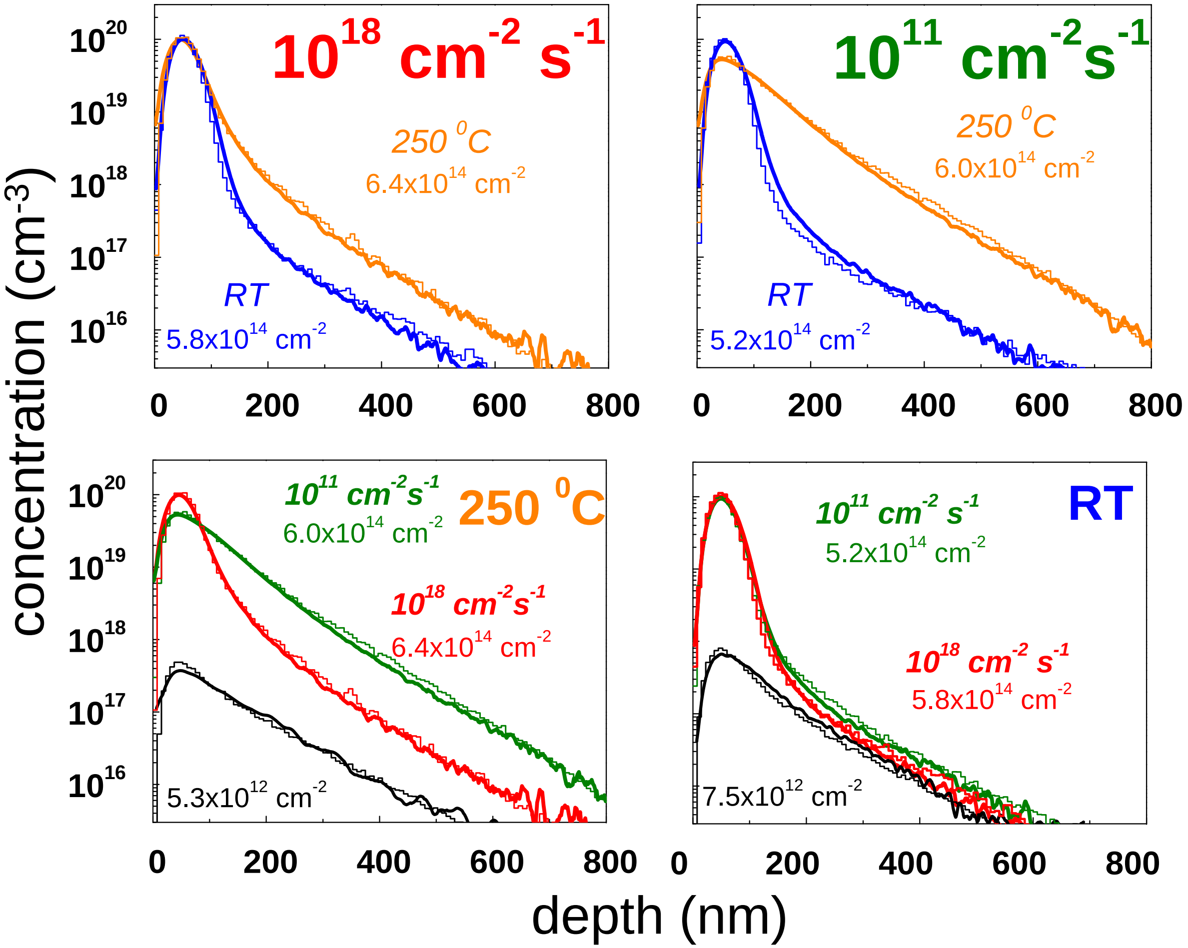
simulation results vs. exp. data:

competition between **damage buildup** and **dynamic annealing**

70 keV Ge$^+$ into (100) Si, **0^0 tilt**

Focused Ion Beam (FIB) implantation





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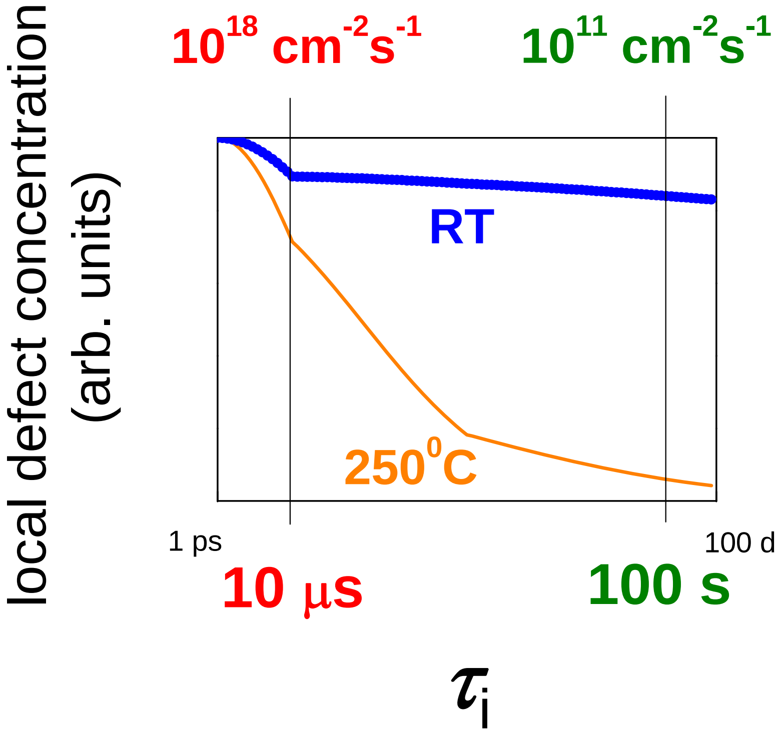
qualitative explanation:

local defect reduction between consecutive ion impacts

τ_i : period between consecutive ion impacts into a target region (cross section σ_0) where the amount of nuclear energy deposition per atom is larger than a critical value E_c

$$\tau_i = \frac{1}{\dot{D}\,\sigma_0} \qquad \sigma_0 = \frac{S_n}{E_c}$$



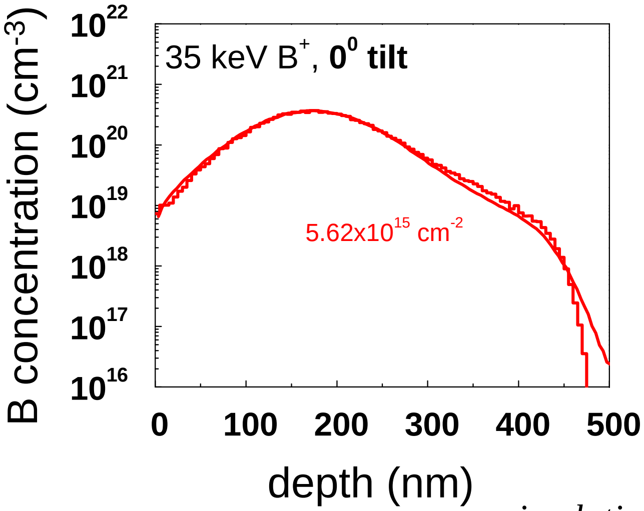
example: multiple implantations

dependence on the implantation sequence

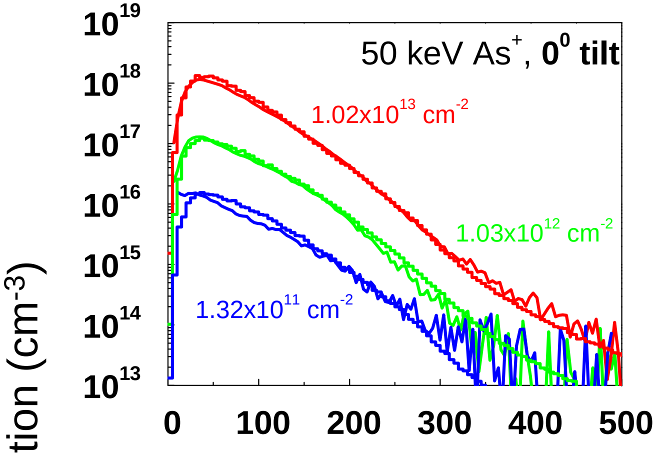
influence of pre-damage

sequence 1:

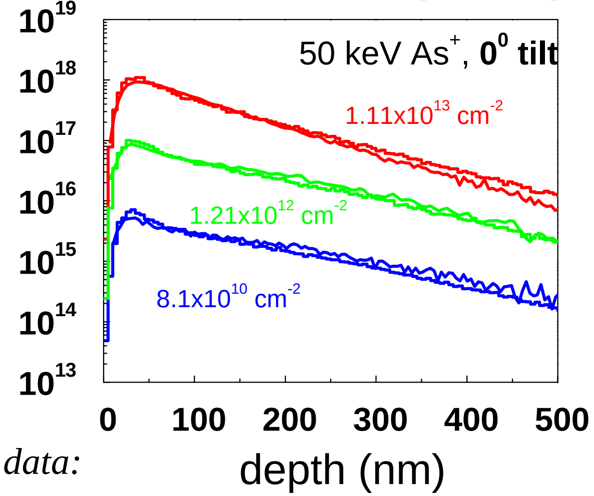
first implantation: B



second implantation: As

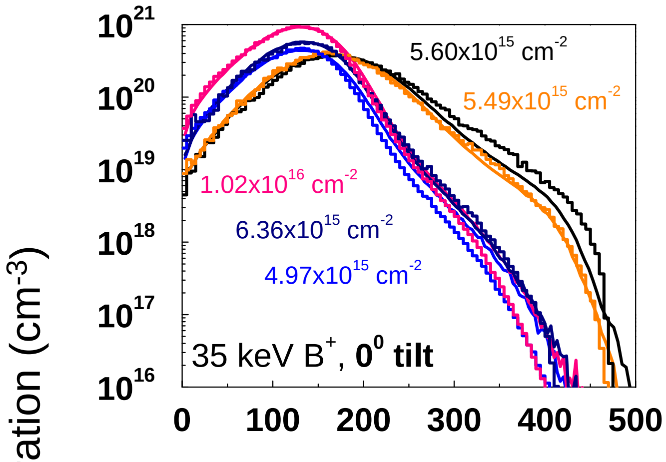


comparison with As profiles obtained without B pre-implantation:



simulation results vs. exp. data:

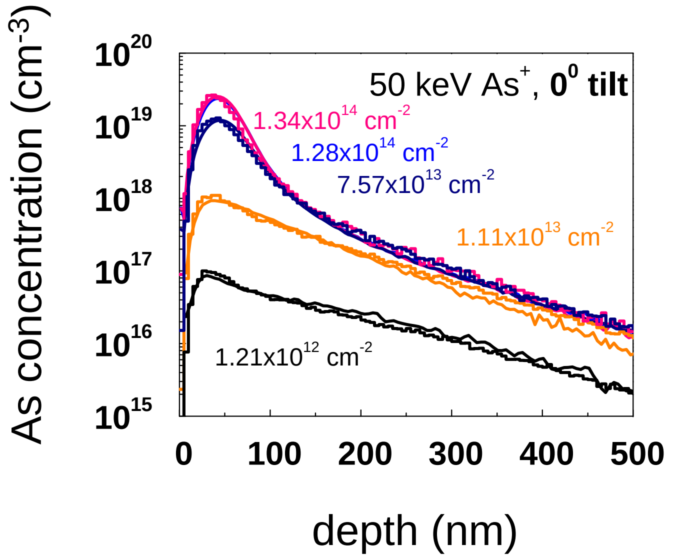
second implantation: B



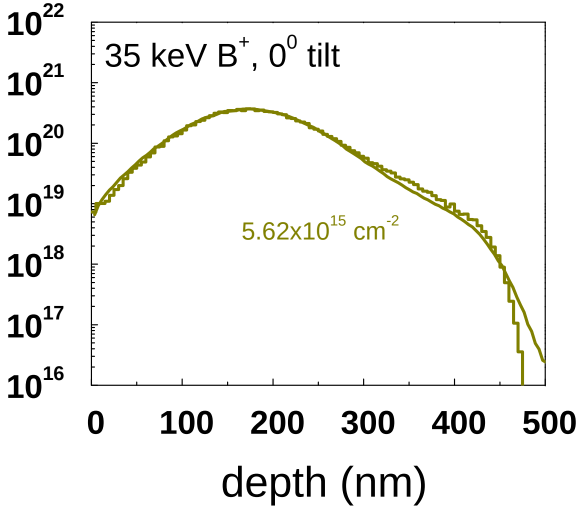
sequence 2:

simulation results vs. exp. data:

first implantation: As



comparison with a B profile obtained without As pre-implantation:



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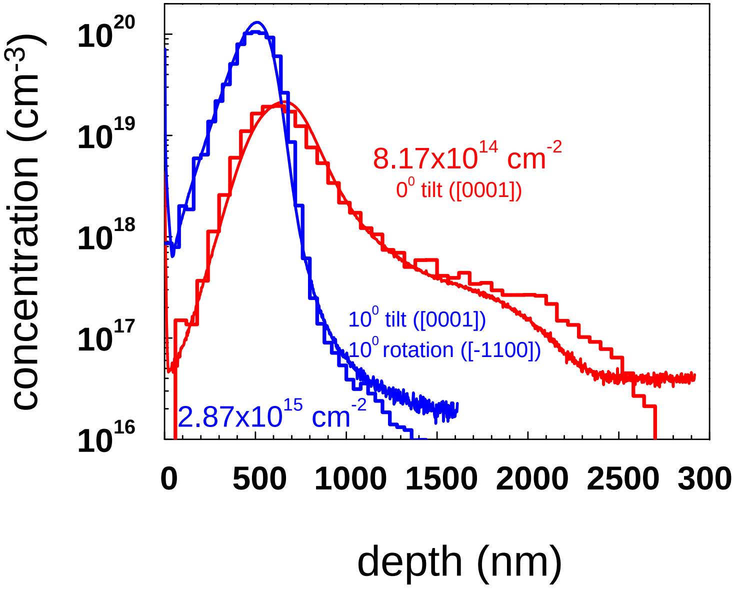
example: implantation into SiC and Ge

simulation results vs. exp. data:

SiC

450 keV Al$^+$ into (0001) 6H-SiC



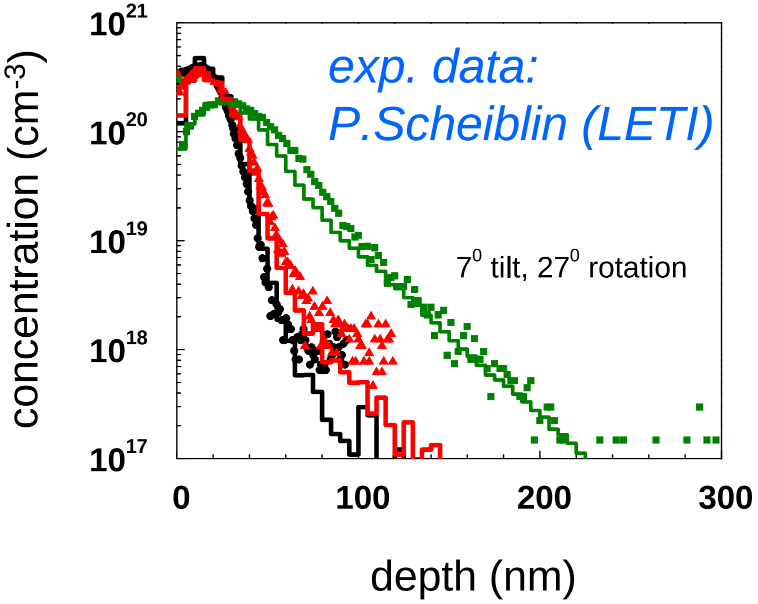
Ge

30 keV As$^+$

18 keV P$^+$

10 keV B$^+$

10^{15} cm^{-2} into (100) Ge



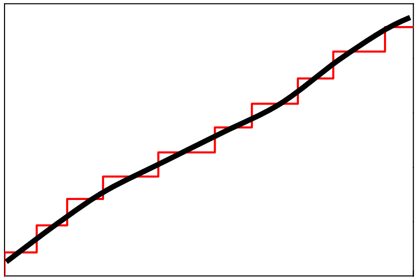
model for damage buildup and dynamic annealing used in Crystal-TRIM

(atomic) damage probability

$p_d(t)$

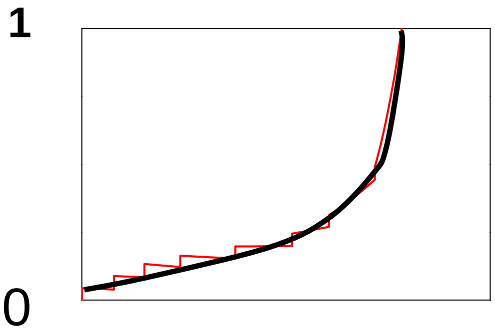
nuclear energy deposition per atom

$E_n^A(t)$

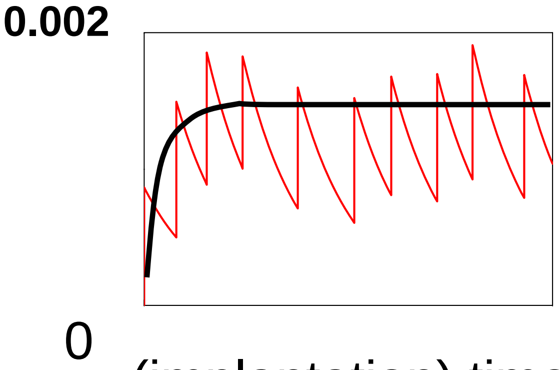


(implantation) time

damage buildup

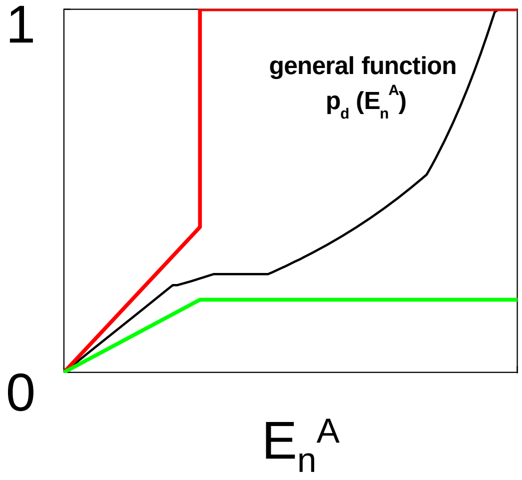


dynamic annealing



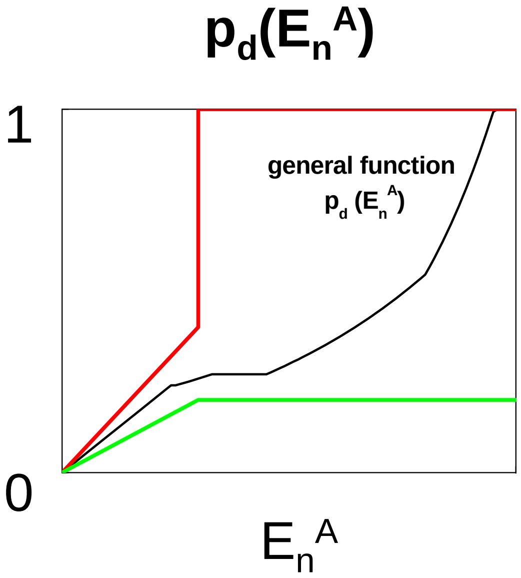
(implantation) time

$p_d(E_n^A)$



only 2 parameters,
dependent on:
- *ion species*
- *temperature*
- *dose rate*

RT implantation into Si, dose rate < 10^{14} cm^{-2} s^{-1}:



the two parameters

linear increase: c_{lin}

threshold value: c_{th}

depend on ion species or

on the <u>morphology of the as-implanted damage</u>

damage accumulation

BF_2^+: $c_{lin} = 0.0045\ eV^{-1}$, $c_{th} = 0.1$

P^+: $c_{lin} = 0.0053\ eV^{-1}$, $c_{th} = 0.1$

As^+, Ge^+, In^+, Sb^+:

$c_{lin} = 0.008\text{-}0.011\ eV^{-1}$, $c_{th} = 0.05\text{-}0.12$

dynamic annealing

B^+: $c_{lin} = 0.0016\ eV^{-1}$, $c_{th} = 0.01$