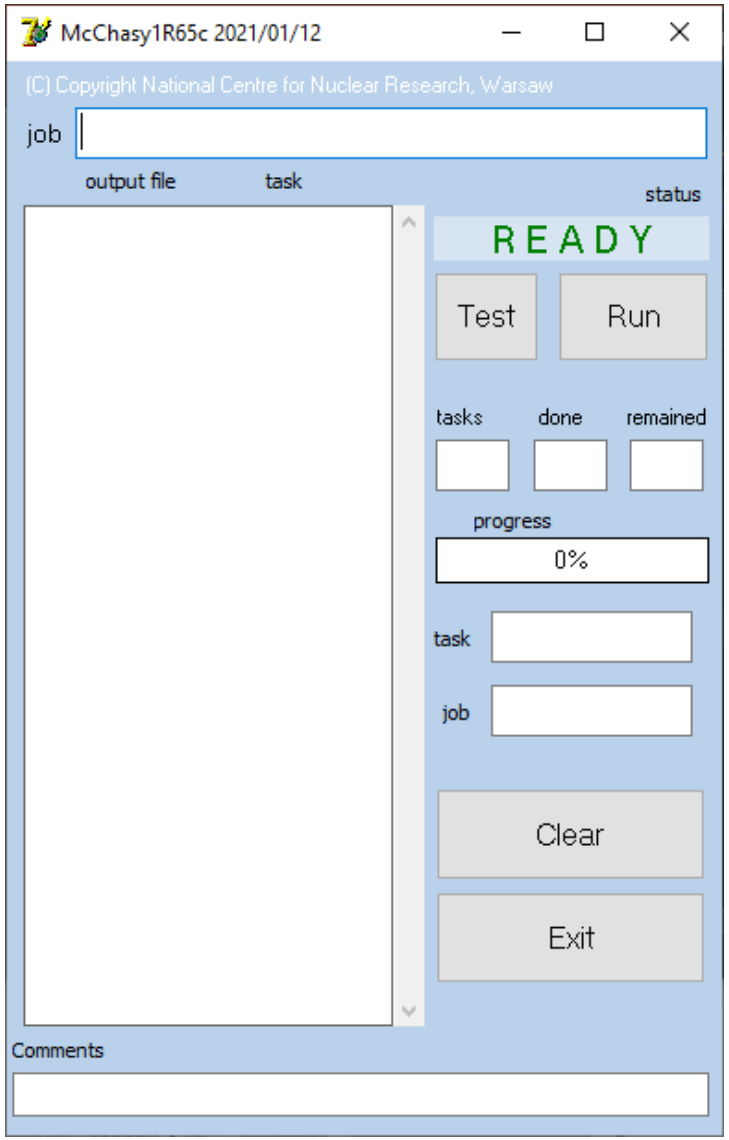
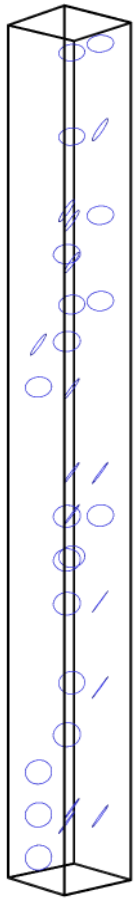
McChasy (**M**onte **C**arlo **CHA**nneling **SY**mulation) – home page



McChasy1	McChasy2
• **Monte Carlo simulations of the ion channeling process**	
• Small structures (<10^2 atoms) composed of monoatomic layers	• Large structures (~10^8 atoms) produced using Molecular Dynamics.
• Displacements due to thermal vibrations or defects applied ‚in-situ' (during ongoing simulations) according to previously implemented models	• Displacements due to thermal vibrations or defects applied using the ATOMSK® or LAMMPS® codes.
• Download the most recent version **here**.	• Available upon collaboration: **contact us**.



Read more about ion channeling and McChasy

- ✓ **Dr. Lech Nowicki –** creator and main developer until 2017 (McChasy1) and 2022 (McChasy2)
- ✓ **Dr. Cyprian Mieszczyński** – developer of nuclear reactions in McChasy1 and current developer of McChasy2
- ✓ **Dr. Przemysław Jóźwik** – developer of dislocations and dislocation loops in McChasy1 and its current developer

McChasy – **M**onte **C**arlo **CHA**nneling **SY**mulation

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    2. Dechanneling vs. direct backscattering
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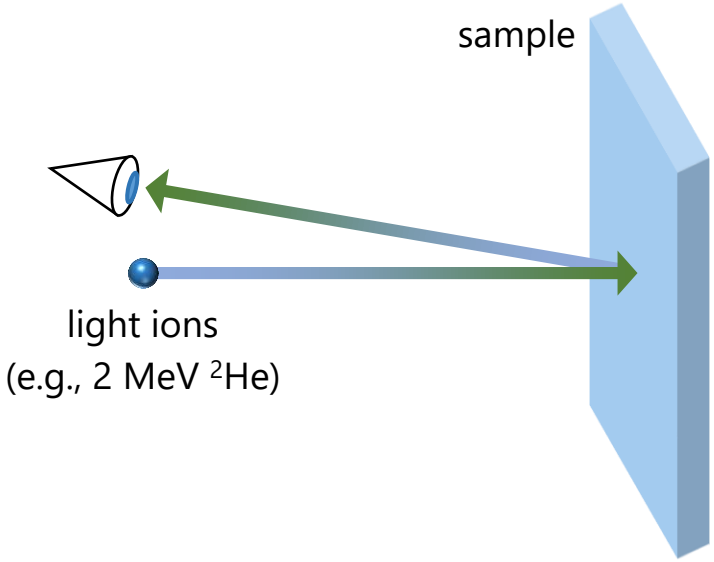
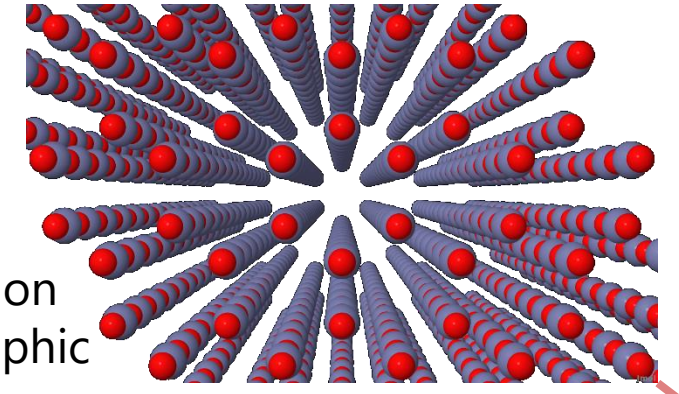
MOTIVATION. Ion channeling

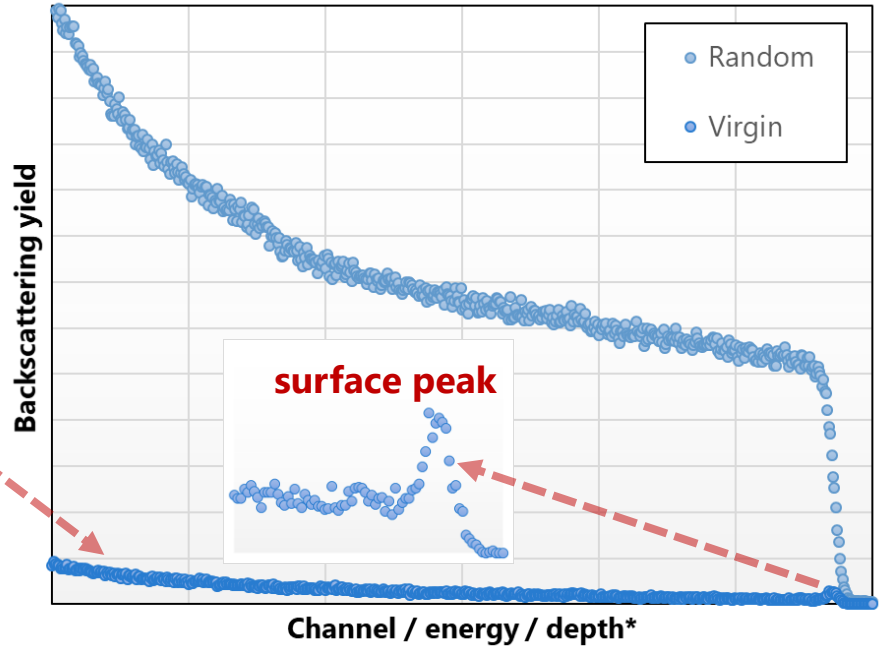


Rutherford Backscattering Spectrometry (RBS) is an analytical technique used to determine the structure and composition of materials. High energy ions (usually ^{1}H or ^{4}He) impinge on a sample and backscatter from target nuclei due to Coulomb interaction. Their energy spectra (i.e., yield vs. energy) are measured at a given angle of detection (typically between 140° and 170° to provide high mass resolution).

Ion channeling (RBS/C or **cRBS)** is a special mode of **RBS** used to analyze crystalline structures. When the incident ion beam is aligned with a major crystallographic axis, it can penetrate the material up to large depths without being backscattered. The measured yield for a **virgin** (=high-quality as-grown) sample can be 2% of the **random** spectrum, which is usually measured by rotating the sample off the axis.

RBS/channeling (**RBS/C**)



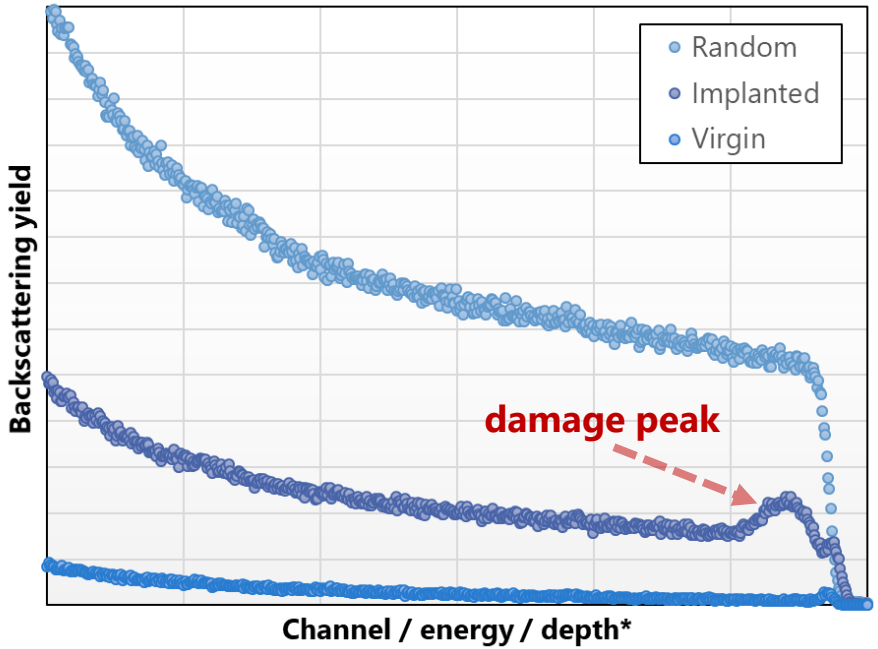


The characteristic **surface peak** in the virgin aligned spectrum is due to backscattering on surface atoms. A part of the beam that was not backscattered from the surface moves deep into the crystal with an oscillatory motion in channels formed by the surrounding atoms

MOTIVATION. Dechanneling vs. direct backscattering

RBS/C is very sensitive to crystallographic defects. It is especially useful to analyze damage created by energetic ion beams, e.g., in the ion implantation process. A typical aligned spectrum recorded for an ion-implanted sample reveals a **damage peak** formed due to **direct backscattering** from interstitial atoms or amorphous regions. However, the yield behind the peak does not reach the virgin level. This is due to **dechanneling** that disrupts the ion channeling and leads to the backscattering in the deeper regions of the sample.

The probability of **dechanneling** depends on the type of defect and the energy of the ion. Therefore, it is challenging to obtain information about defect types and their depth distribution from a single RBS/C spectrum in an unambiguous way.



[1] A. Vantomme, 50 years of ion channeling in materials science, Nuclear Instruments and Methods in Physics Research, Section B: Beam Interactions with Materials and Atoms. 371 (2016) 12–26. https://doi.org/10.1016/j.nimb.2015.11.035.

MOTIVATION. Dechanneling vs. energy of the ion

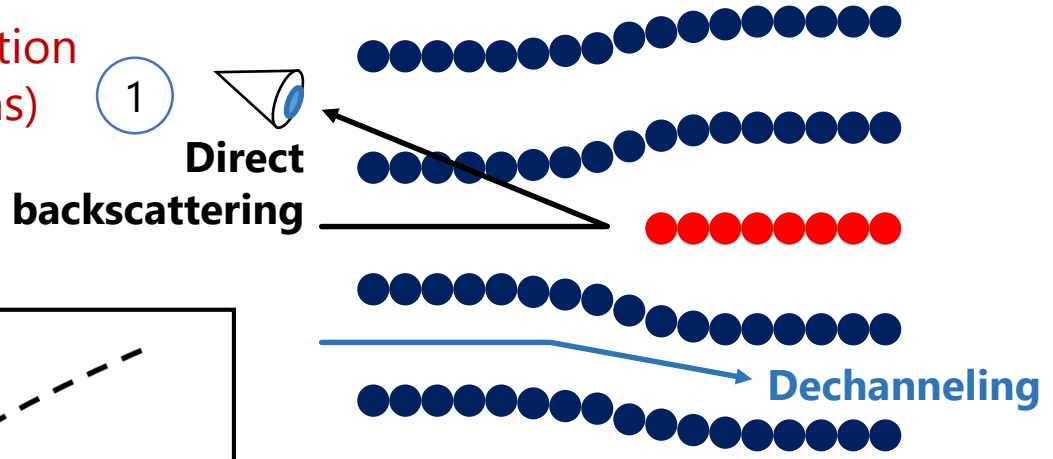
Dechanneling factor

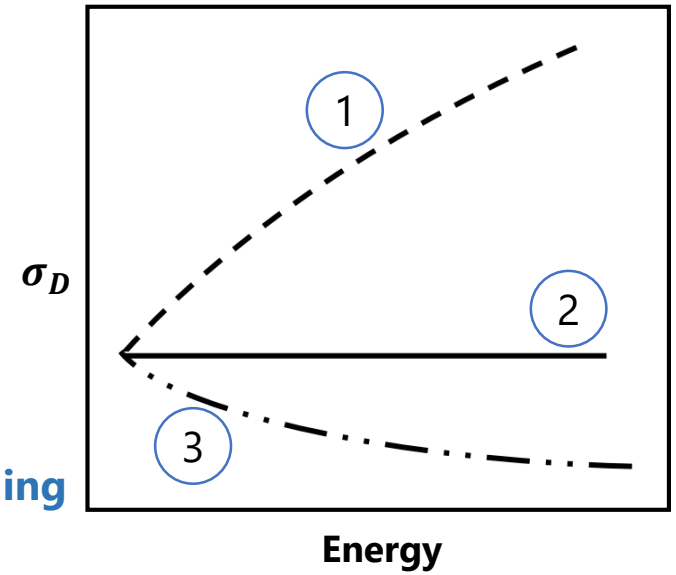
Probability of dechanneling per unit depth

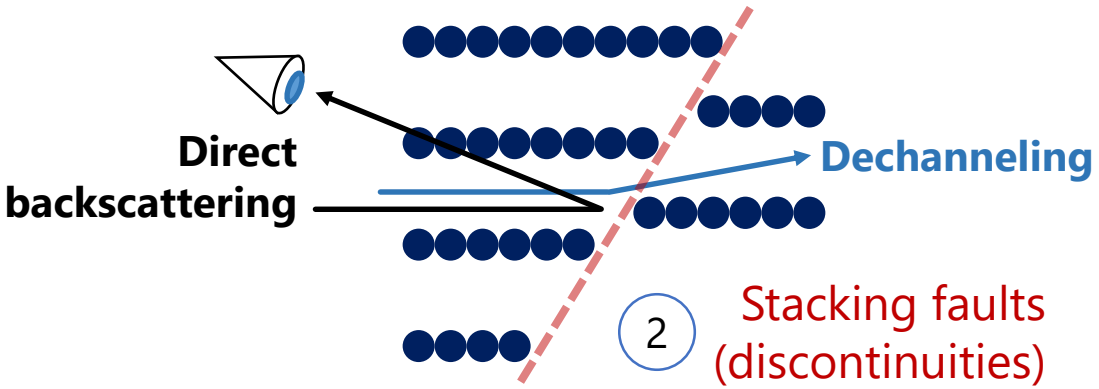
$$\frac{dP_D}{dz} = \sigma_D n_D(z)$$

Defect density

Dislocations, dislocation loops (tensed regions)

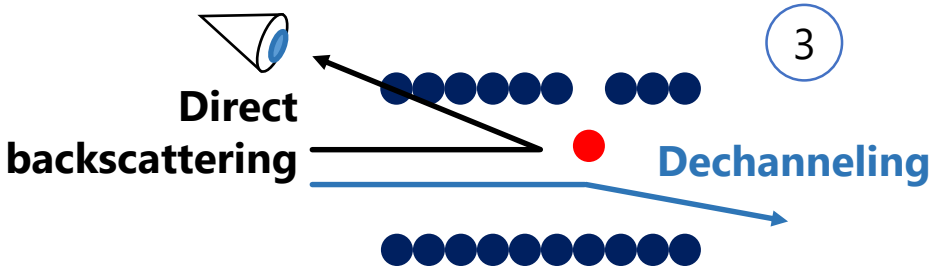






Stacking faults (discontinuities)

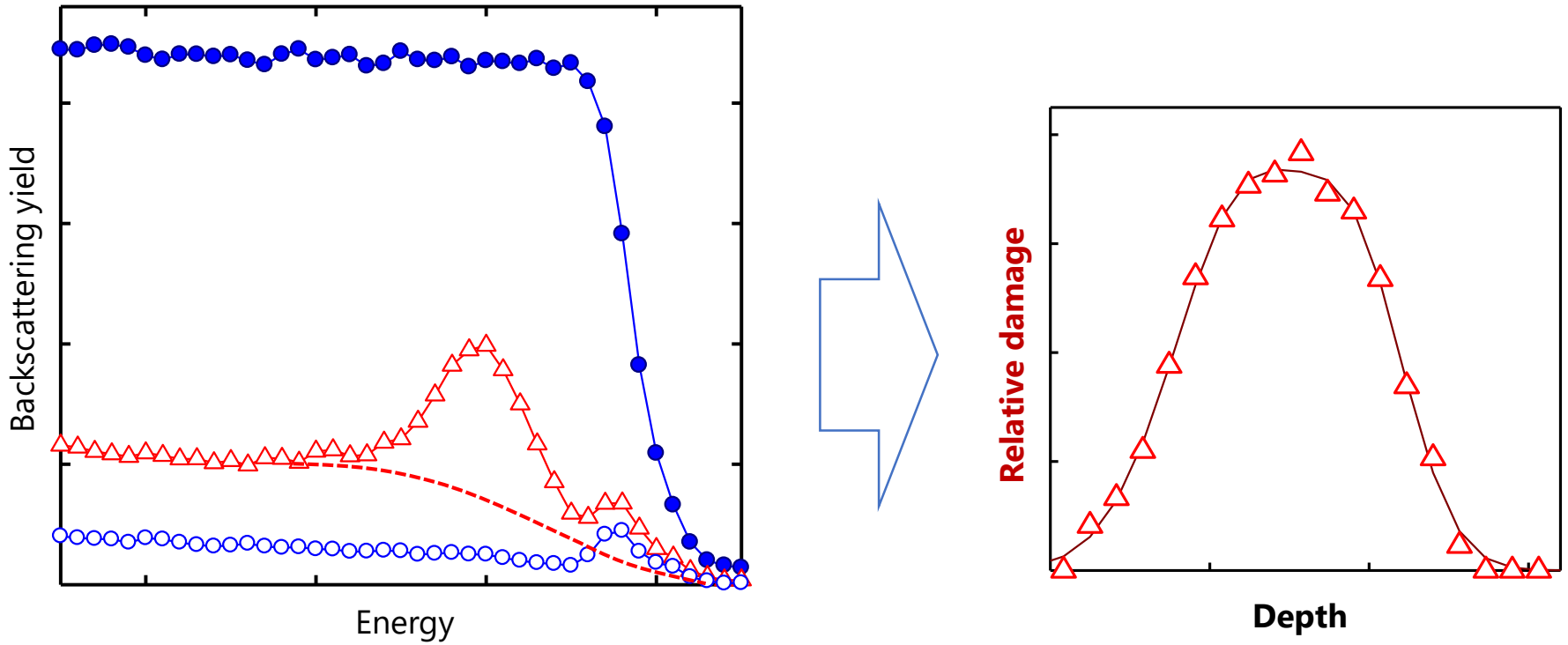
Interstitials, amorphous clasters (point scattering centers)



[2] L.C. Feldman, J.W. Mayer, S.T. Picraux, Materials Analysis by Ion Channeling: Submicron Crystallography, Academic Press, New York, 1982.

MOTIVATION. Two-beam approximation

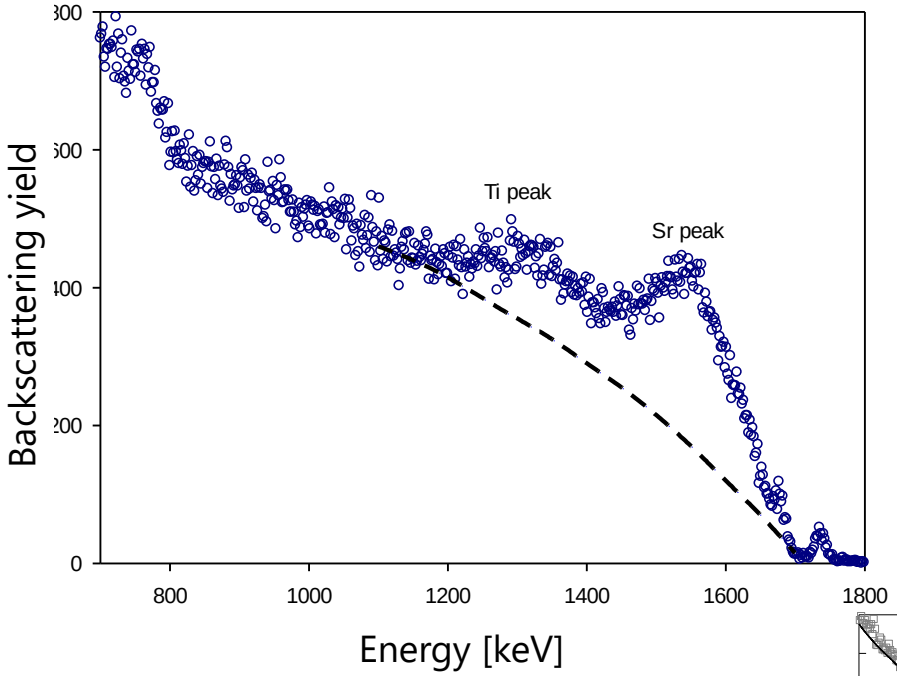
Two Beam Approximation (TBA) is commonly used to extract damage profiles from RBS/C spectra. **TBA** assumes that the analyzing ion beam consists of two fractions: random and channeled ones. However, there is no analytical possibility to distinguish between dechanneling and direct backscattering, both leading to an increase in the random fraction at the expense of the channeling once. Because of that fact, defect profiles extracted using the TBA are usually characterized as "relative damage" assuming the presence of point defects only, with no information about extended ones (e.g., dislocations or dislocation loops).



[3] E. Bøgh, Defect studies in crystals by means of channeling, Canadian Journal of Physics. 46 (1968) 653–662. https://doi.org/10.1139/p68-081.

MOTIVATION. Ion channeling: dechanneling challenge

320 keV Ar-implanted $SrTiO_3$

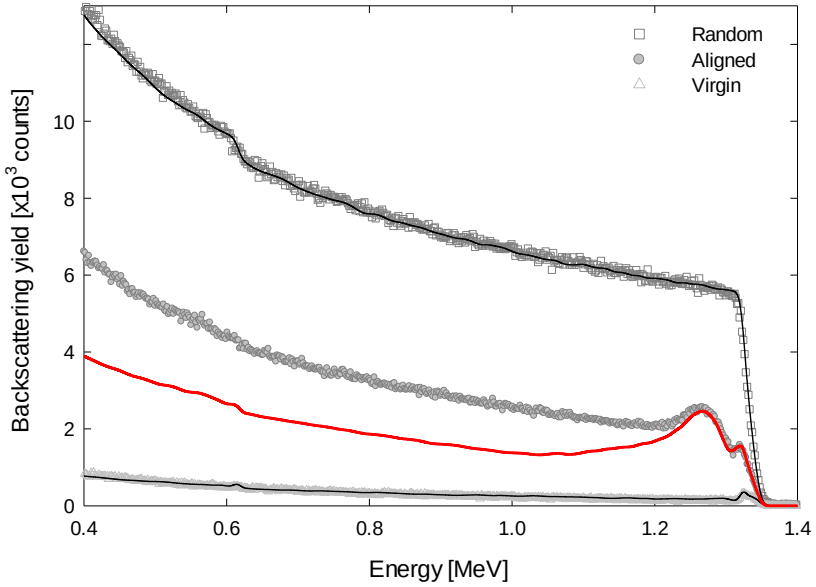


TBA fails in many cases, e.g.:

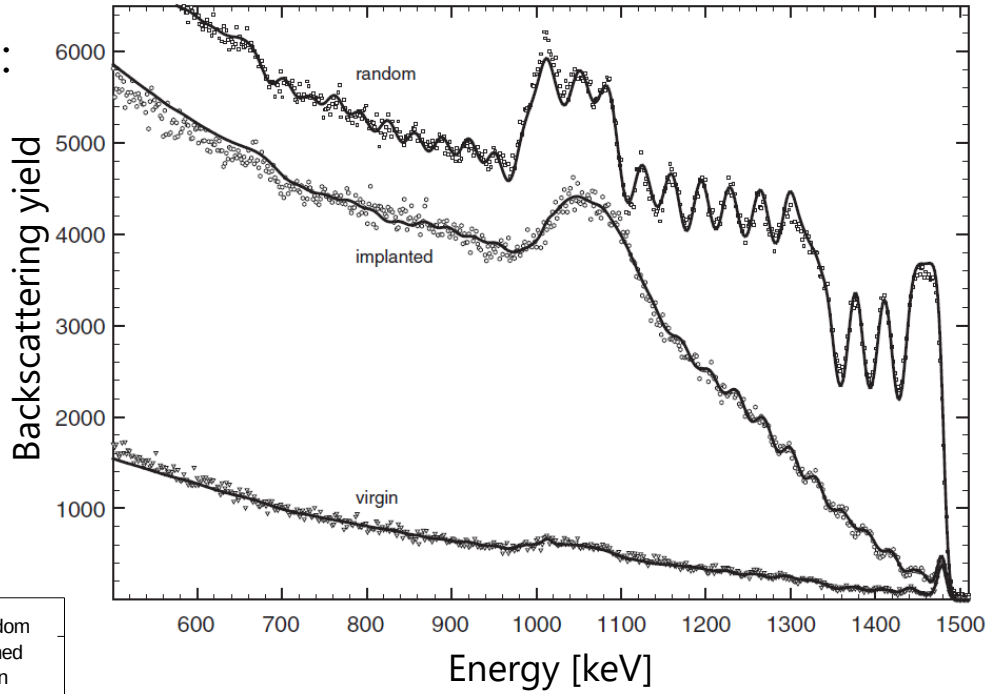
← complex structures

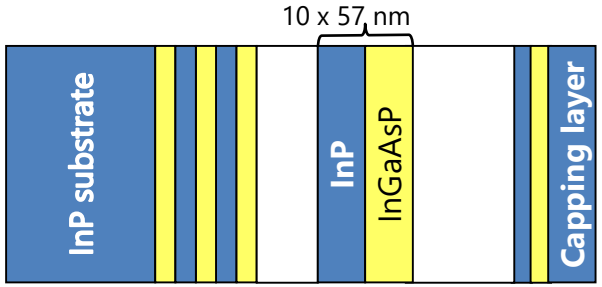
→ multi-layers

↓ extended defects present (increasing dechanneling level)

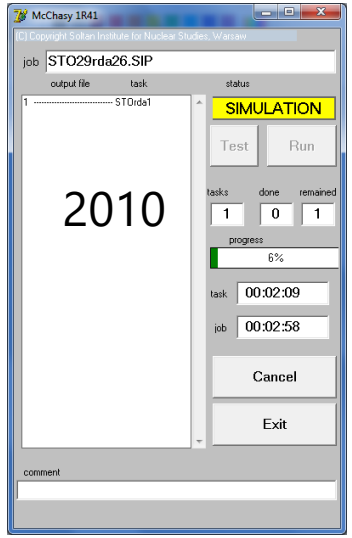


Superlattice 10x($InP/In_{0.54}Ga_{0.46}As_{0.94}P_{0.06}$

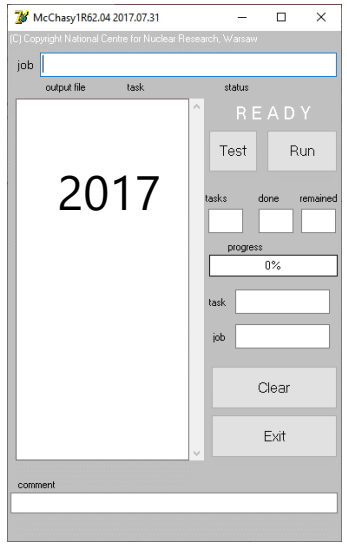




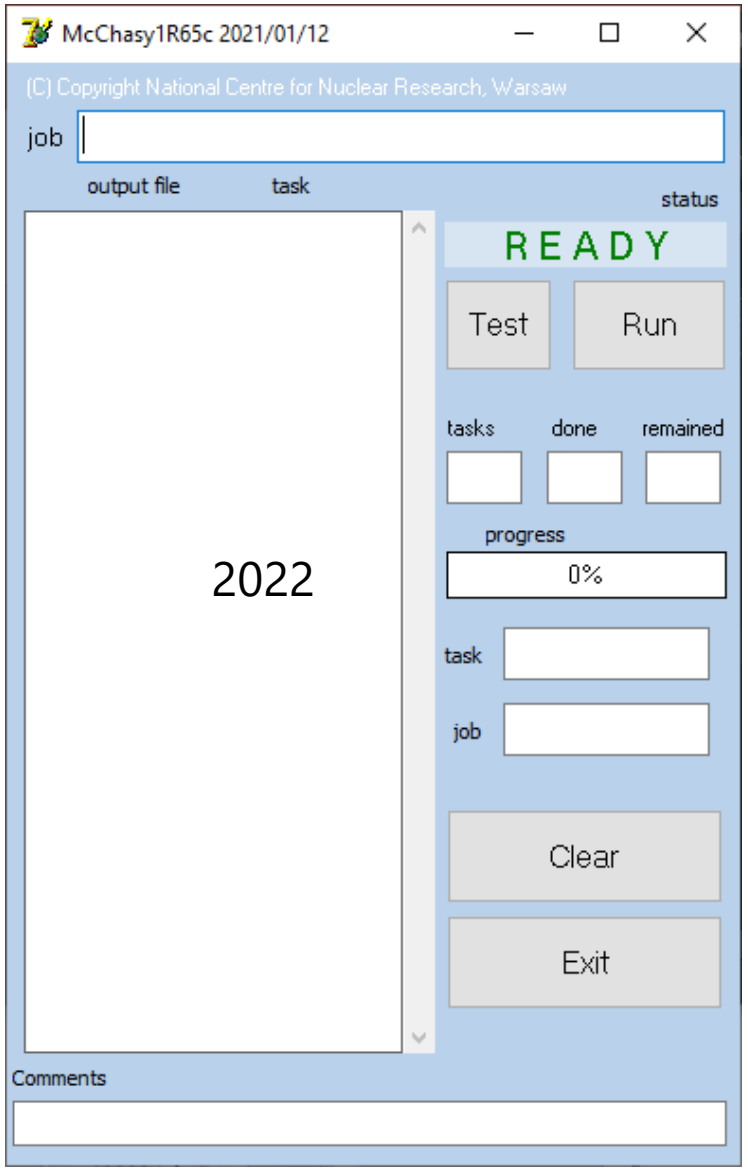
McChasy - Overview



2010

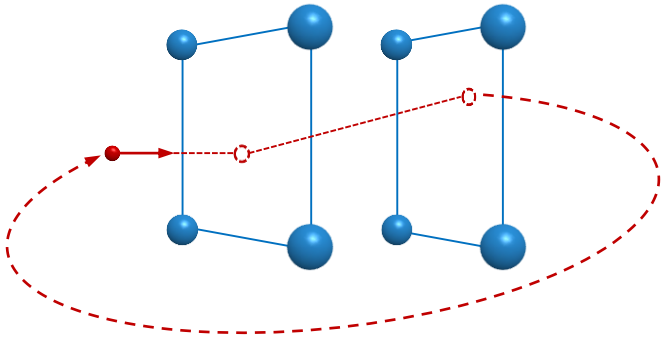


2017



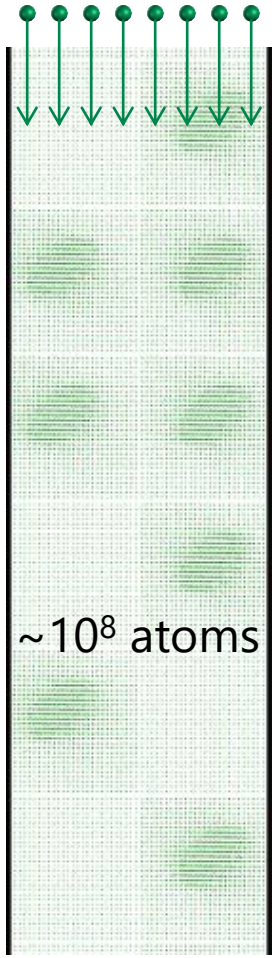
2022

McChasy-1

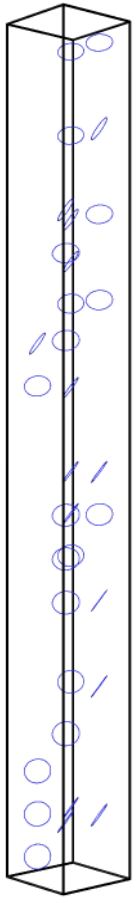


<~10^2 atoms

McChasy-2



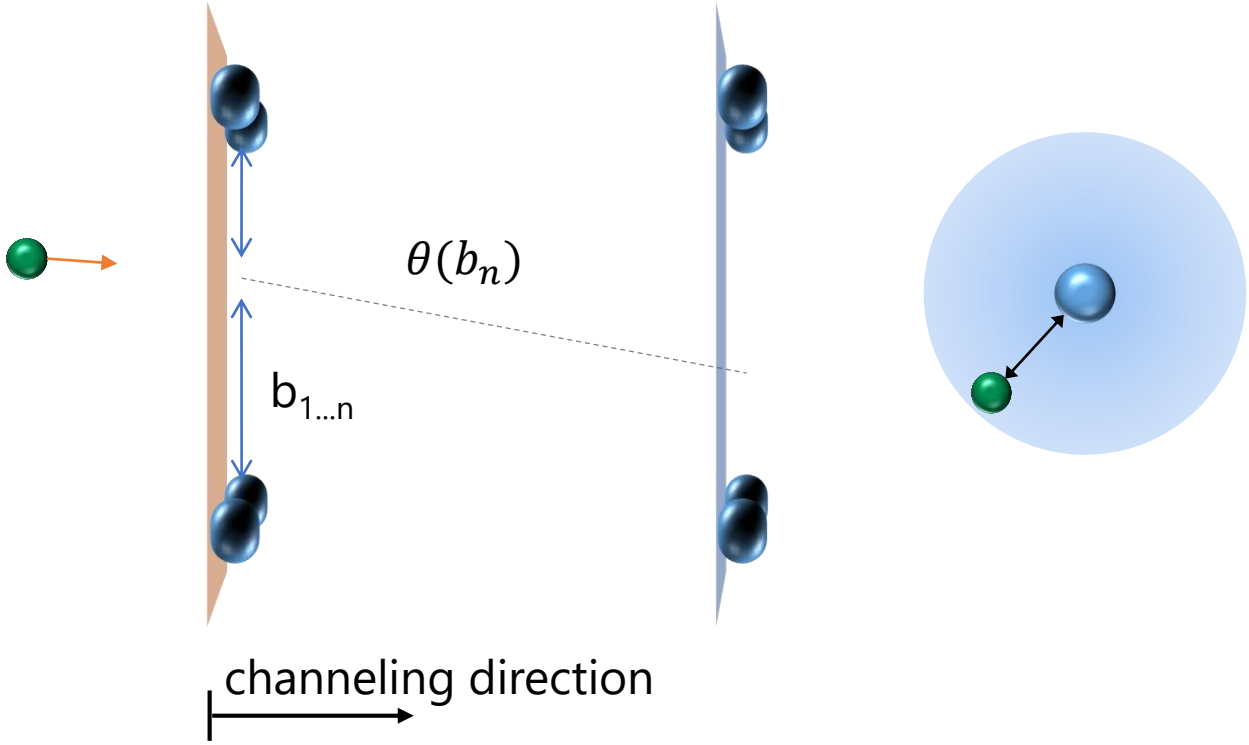
~10^8 atoms

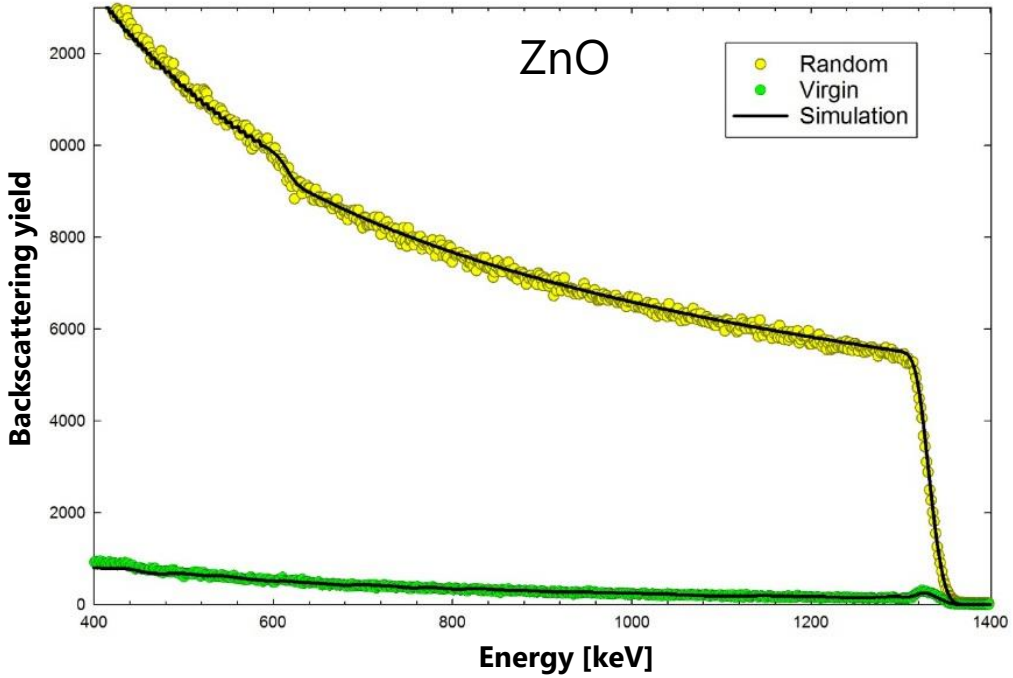


Monte Carlo (MC) simulations are a solution to the problem of different types of defects

McChasy - Overview

As proposed by **Barrett**, the movement of probing ions in crystalline structures can be reproduced while the scattering probability can be sampled → **Nuclear Encounter Probability (NEP)**. Its distribution can be eventually transformed into an RBS spectrum. This approach is the engine of the **McChasy** code.





[4] J.H. Barrett, Monte carlo channeling calculations, Physical Review B. 3 (1971) 1527–1547. https://doi.org/10.1103/PhysRevB.3.1527.

McChasy-1. Specification

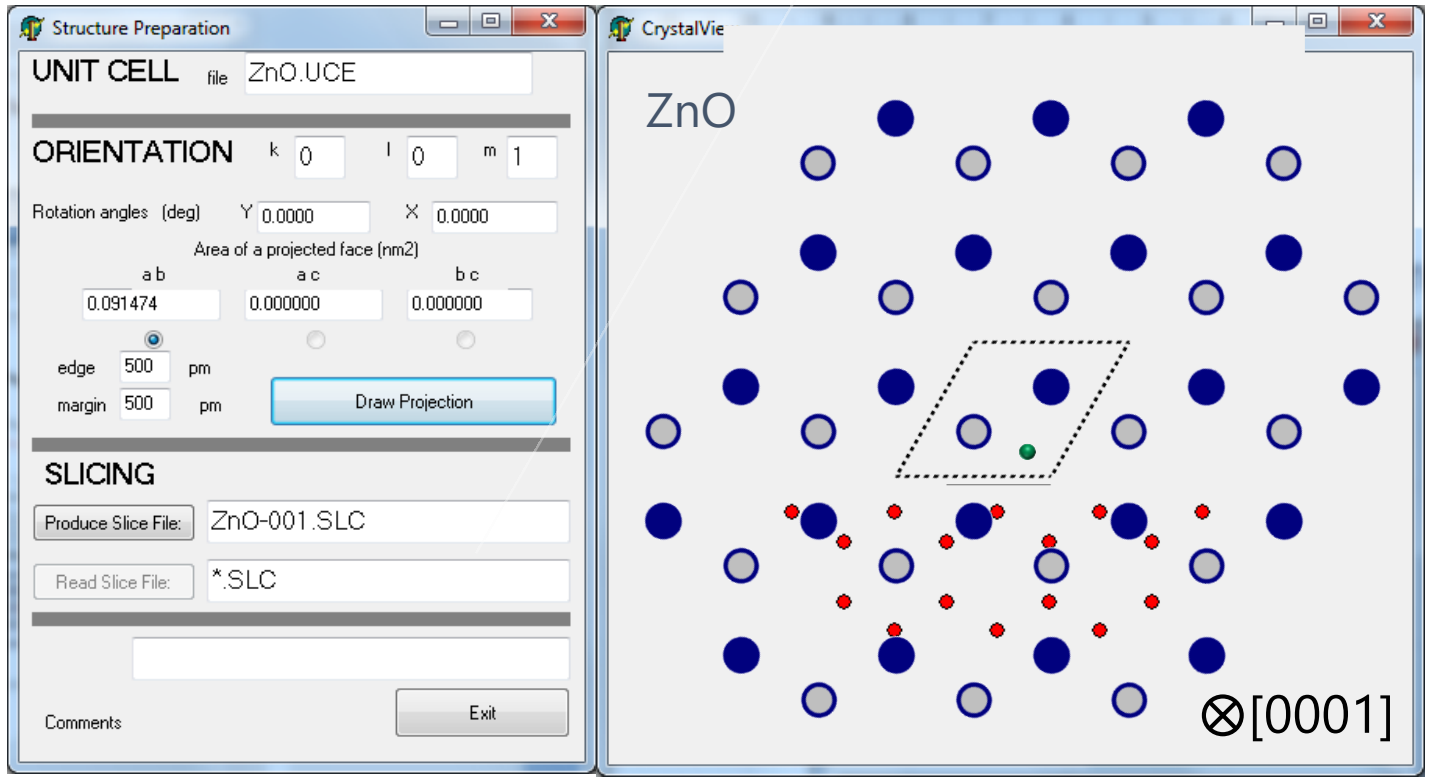
- Reproduces RBS/C spectra using MC simulations.
- Provides angular scans.
- Can be launched on typical PCs.

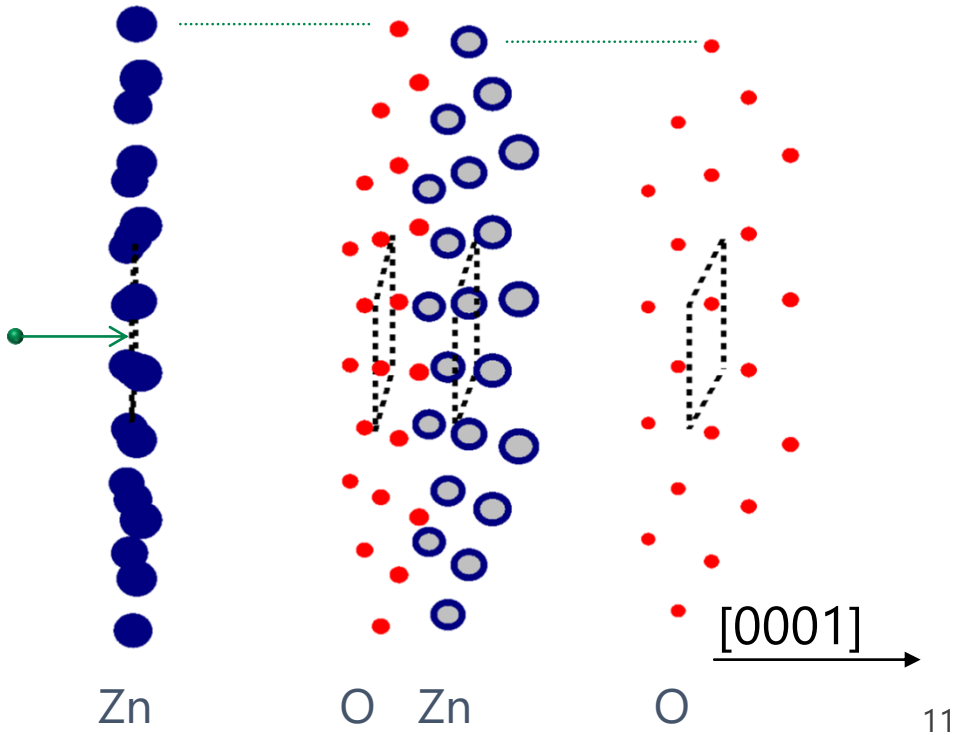
- Projectiles: ^{4}He, ^{1}H, ^{2}H
- Projectile energy: 0.8 – 5.0 MeV
- Crystal stryctures:
  - elements: Si, Sn, Al, Cu, Au, Fe, Nb, …
  - compounds: (Al,Ga,In) × (N,P,As,Sb), ZrO_2, $MgAl_2O_4$, U_xO_y, Al_2O_3, MnO_3, ZnO, $SrTiO_3$…
- Channeling axes: [001], [011], [111] – for cubic
  [0001] – for hexagonal
  [001] – for perovskites

- Potential: ZBL
- Non-Rutherford resonances: possible
- Energy loss: RUMP or TRIM
- Electron density: Lindhard approach
- Thermal vibrations: 3D Gaussian probability

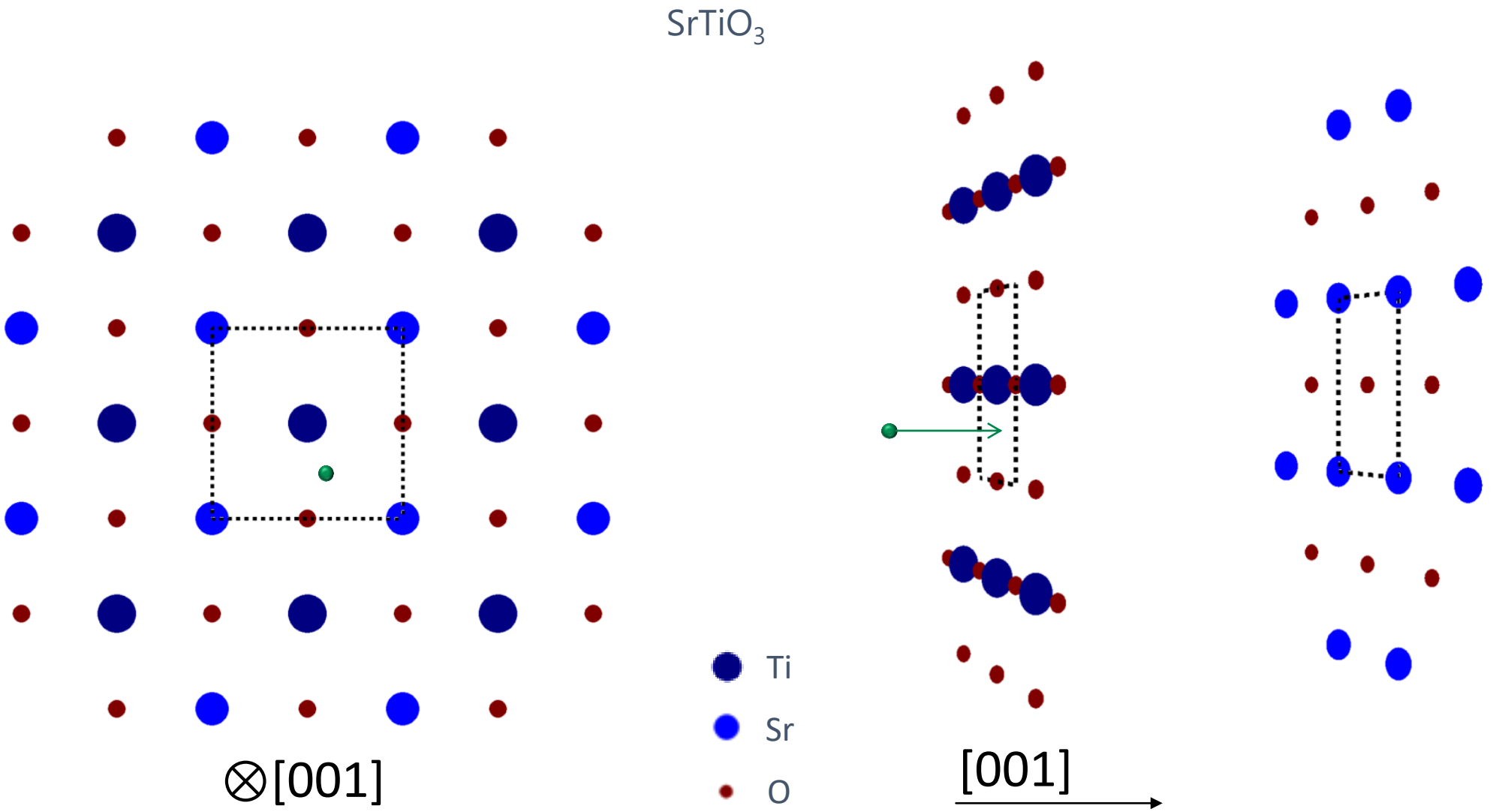
Working with McChasy-1. Structure preparation.

McChasy uses the **Planar Scattering Approximation (PSA)**. Structures used for MC simulations are composed of monolayers of atoms. A variety of structures in different channeling directions are already available for use while any new one can be created on demand using an associated program called Structure Preparation. During ongoing simulations, **McChasy** calculates interactions of a probing ion with all the atoms of each monolayer and determines the scattering probability.

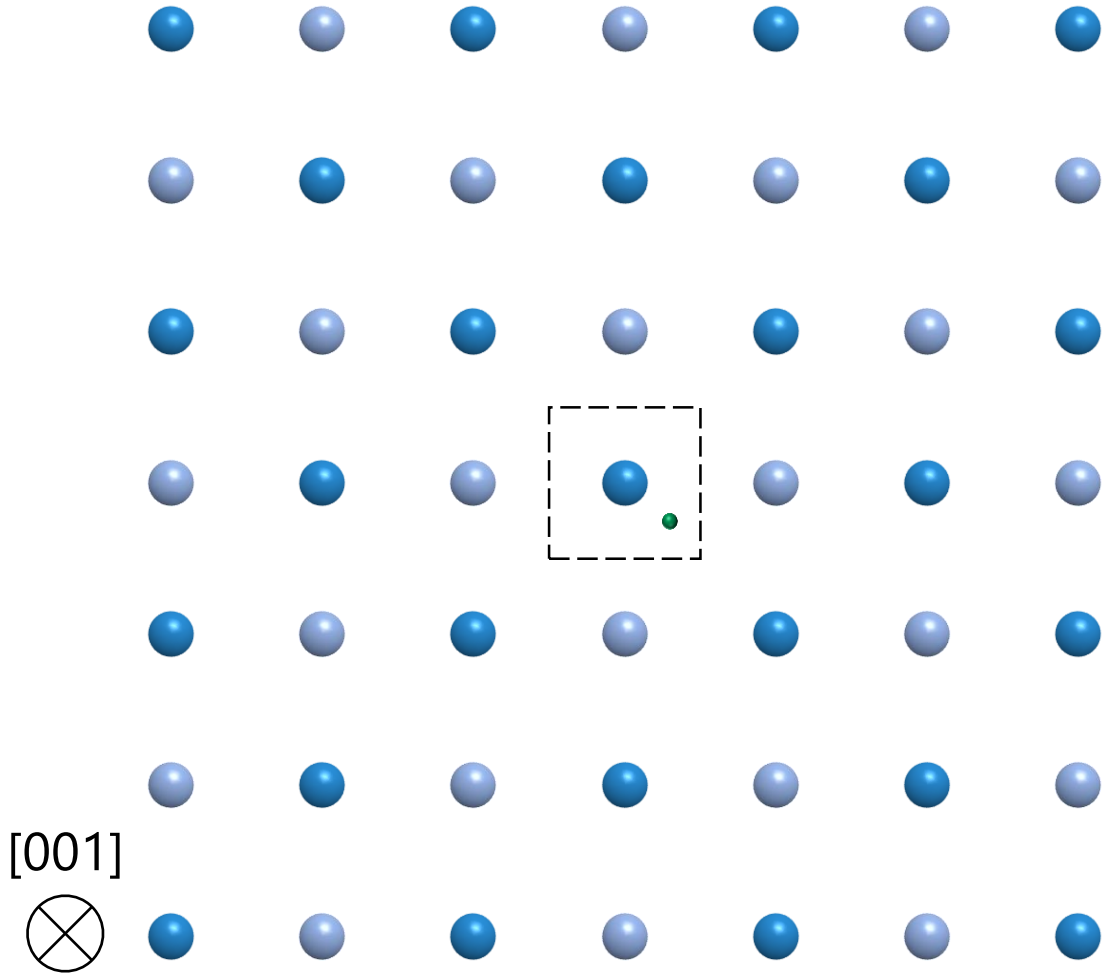




Working with McChasy-1. Structure preparation.

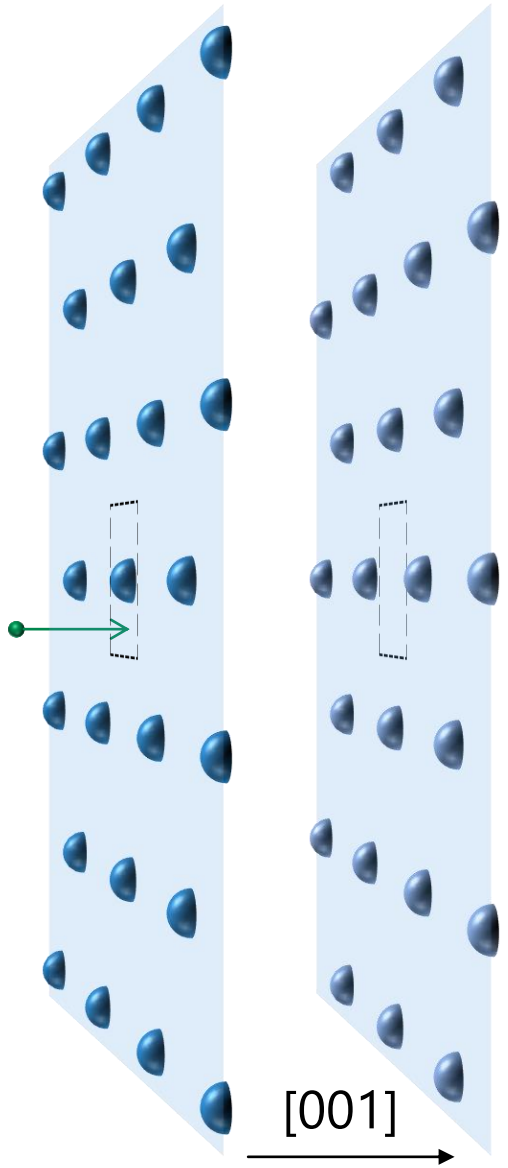


Working with McChasy-1. Structure preparation.



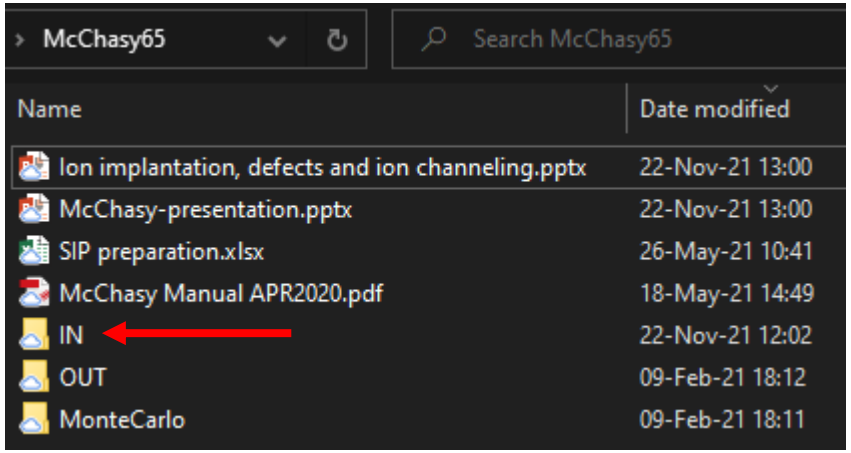
Ni

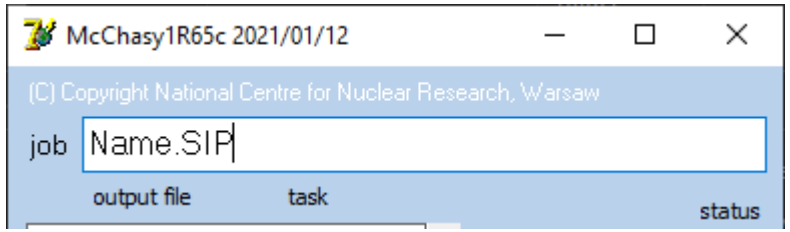
<~10^2 atoms



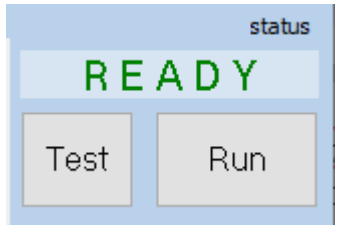
Working with McChasy-1. Input file preparation

McChasy folder contains three subfolders that must not be removed or renamed: **IN**, **OUT**, and **MonteCarlo**. To begin your work with **McChasy**, you need to prepare an input file (*Name.SIP* – Simple Input Protocol) that must be saved in the **IN** folder. Follow the instructions and examples that are provided in the most recent *Manual* file that is located in the main **McChasy** folder. You will find the executive file of **McChasy** in the MonteCarlo folder (e.g., *Mc1R65.exe*). The results of simulations are saved in the subfolder OUT*Name*.





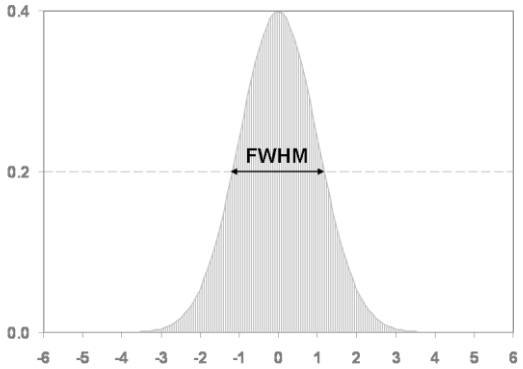
To start simulations, type the name of your SIP file in the job box (the extension '*.SIP*' is optional – it will be added automatically if missing).



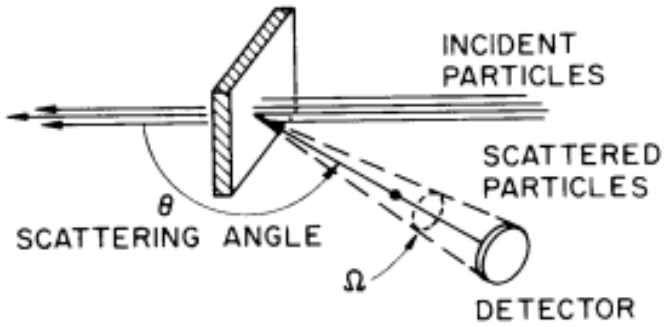
For a newly created SIP file, it is a good idea to test it using the Test button. If no errors are found, you can click on the Run button. When you modify your SIP file slightly, you can skip the test and go directly to the Run option.

Working with McChasy-1. Input file preparation

Selected typical commands used in SIP files are shown and described below. You can use an Excel file called SIP preparation.xlsx to prepare SIP files. You just need to highlight the desired area (five columns up to the last EXE command), copy it, and paste it as a whole into the SIP file. You can follow the shortcut: Go to cell A1, hold Ctrl+Shift and type Arrow right, then Arrow down.



Command	Value		Comment
ENE	2000		projectile energy [keV]
SCA	165		scattering angle [deg]
RES	15		energy resolution *fwhm* [keV]
BEC	2.40	122	energy calibration: channel width and offset [keV]
PAR	10000		number of particles
TGT	ZnO		name of the structure
OMC	1.9	40	detection solid angle [mSr] and integrated charge [μC]
VIB	Zn	9.5	amplitude of thermal vibrations [pm]
THI	1700		thickness [nm]
KLM	001		channeling axis
EXE	TaskName		execute a task



Working with McChasy-1. Results

times.TXT

TaskNum	TName	TaskTime
1	simRDA	00:32:03
2	simDIS	00:32:26
TotalJobTime:		01:04:41

Unless otherwise indicated, at least three files are saved in the subfolder OUT\Name, where Name is the name of the SIP file you used for simulations: a copy of the SIP file, times.TXT, and Name.TXT.

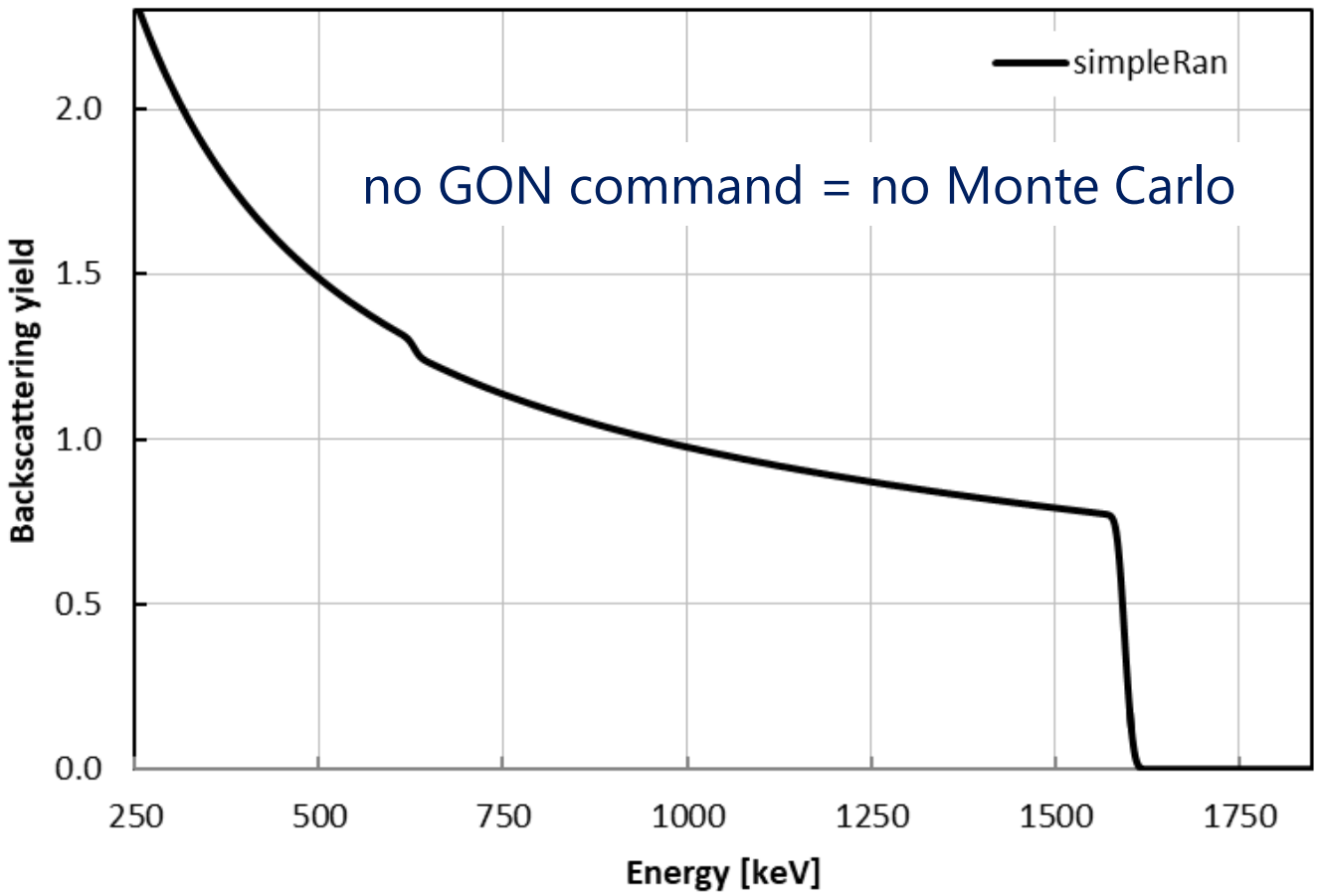
Name.TXT

	simRDA		simDIS	
energy	yield	energy	yield	
1.9340	9.13812E+2	1.9340	4.83048E+2	
3.6950	1.83538E+3	3.6950	9.66971E+2	
5.4560	2.04508E+3	5.4560	1.07700E+3	
7.2170	2.29472E+3	7.2170	1.20798E+3	
8.9780	2.58081E+3	8.9780	1.35813E+3	
10.7390	2.91402E+3	9.7390	1.53305E+3	
…	…	…	…	
	2.77053E+6		1.39876E+6	- SUM
			1.27344E+1	- DIS parameter
			0.00000E+0	- N/A

In the file times.TXT, you can check the duration of the simulations. The relevant simulation results can be found in the file Name.TXT. For each task, two columns are shown: energy (in keV) and backscattering yield (in counts). You can copy and paste the results to any software dedicated to data analysis, e.g., Microsoft Excel, Origin, or SigmaPlot. It is a good idea to associate the result text file with the data analysis software to easily refresh it when you repeat the simulations.

Working with McChasy-1. Examples

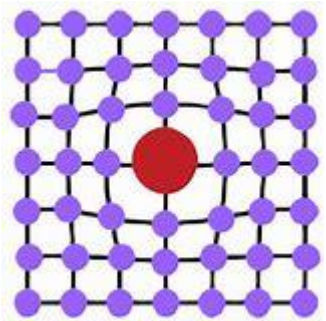
ENE	2000	
SCA	165	
RES	15	
BEC	2.4060	122
PAR	10000	
TGT	ZnO	
OMC	1.9	40
VIB	Zn	9.5
THI	1700	
KLM	001	
EXE	simpleRan	



Models of defects. SUBstitutions

McChasy can substitute target atoms with impurity atoms using a combination of two commands: SUB and SBL. Use SUB to define an element to be substituted and its substitution. SBL is used to define a number of layers for a depth distribution of the substitutional atoms.

```
SUB 1 Zn Er                          - Er substitutes Zn
SBL      10                          - Nº of layers below
***      depth     subst
***      (nm)      1
1        0         0.00
2        20        0.10
3        30        0.33
4        40        0.63
5        50        0.99
6        60        0.70
7        70        0.47
8        80        0.27
9        90        0.05
10       100       0.00
```

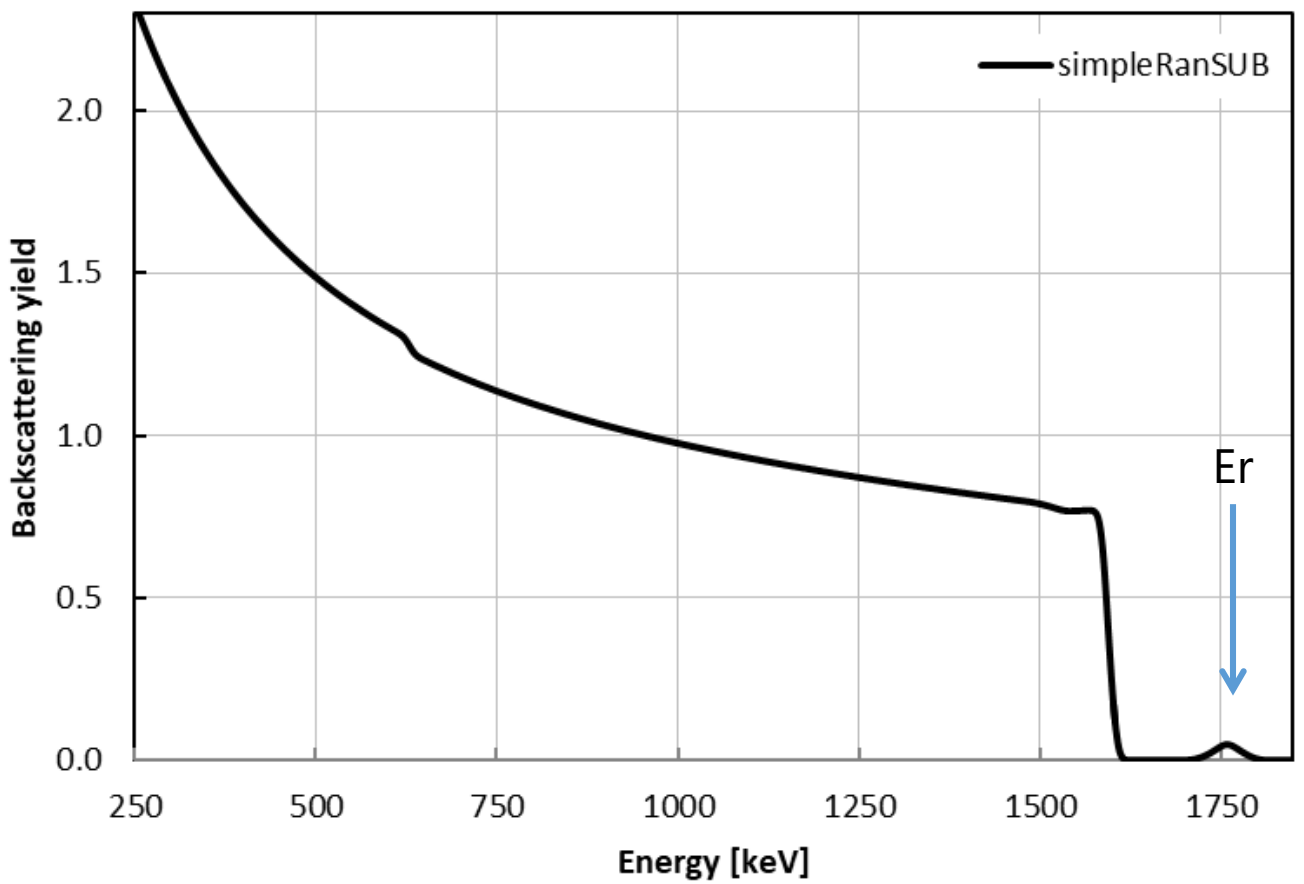


Between 40 and 50 nm from the surface 0.63% of Zn atoms is substituted by Er

```
SUB 1 Zn Er                          - Er substitutes Zn
SUB 2 O Mg                           - Mg substitutes O
SBL      10                          - Nº of layers below
***      depth     subst1    subst2
***      (nm)      1         2
1        0         0.00      0.00
2        20        0.10      0.20
3        30        0.33      0.20
4        40        0.63      0.45
5        50        0.99      0.45
6        60        0.70      0.15
7        70        0.47      0.15
8        80        0.27      0.00
9        90        0.05      0.00
10       100       0.00      0.00
```

Simple random of GaN with Er-SUBstitutions

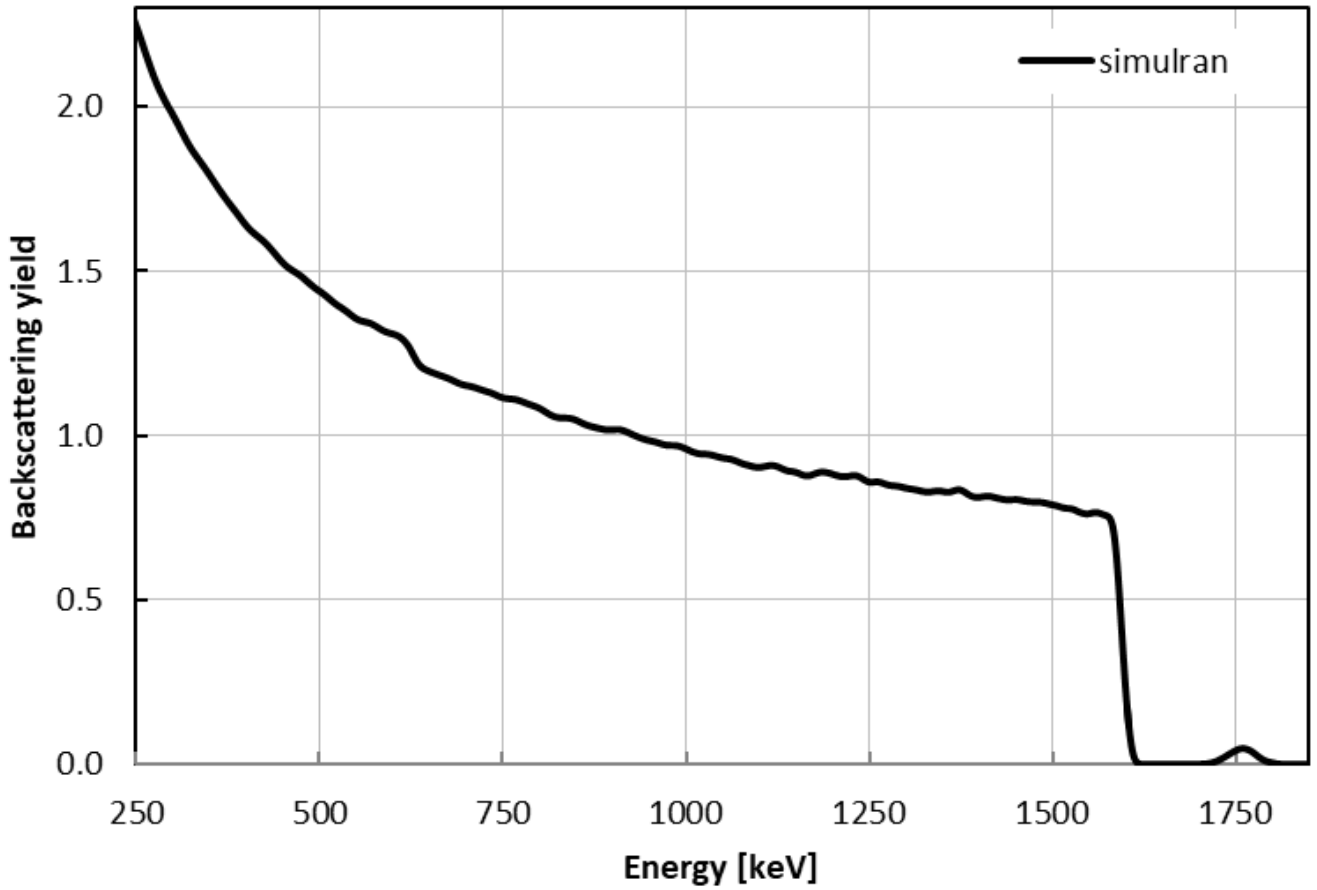
SUB 1 Ga Er		- Er substitutes Zn
SBL	10	- 10 layers
***	depth	subst
***	(nm)	1
1	0	0.00
2	20	0.10
3	30	0.33
4	40	0.63
5	50	0.99
6	60	0.70
7	70	0.47
8	80	0.27
9	90	0.05
10	100	0.00



Simulated random of GaN with Er-SUBstitutions

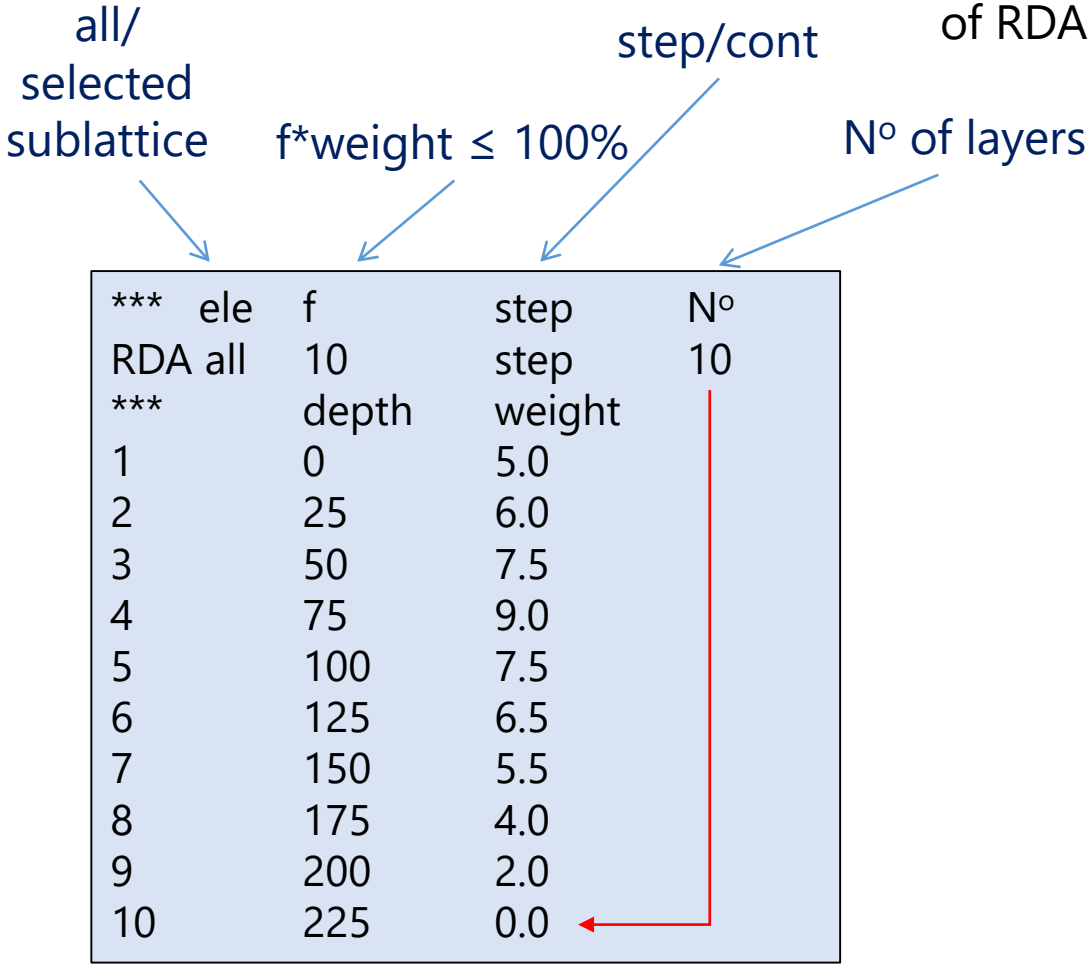
ENE	2000	
SCA	165	
RES	15	
BEC	2.4060	122
PAR	10000	
TGT	ZnO	
OMC	1.9	40
VIB	Zn	9.5
THI	1700	
KLM	001	
GON	rotate 5	
SUB 1 Zn Er		
SBL	10	
***	depth	subst
***	(nm)	1
1	0	0.00
2	20	0.10
	…	…
EXE	simulRan	

The command GON corresponds to a virtual goniometer, as for the real RBS measurements, and also triggers the MC simulations. GON rotate 5 means that a structure is tilted by 5° off the channeling axis and rotated around it (a common way to measure the Random spectrum).

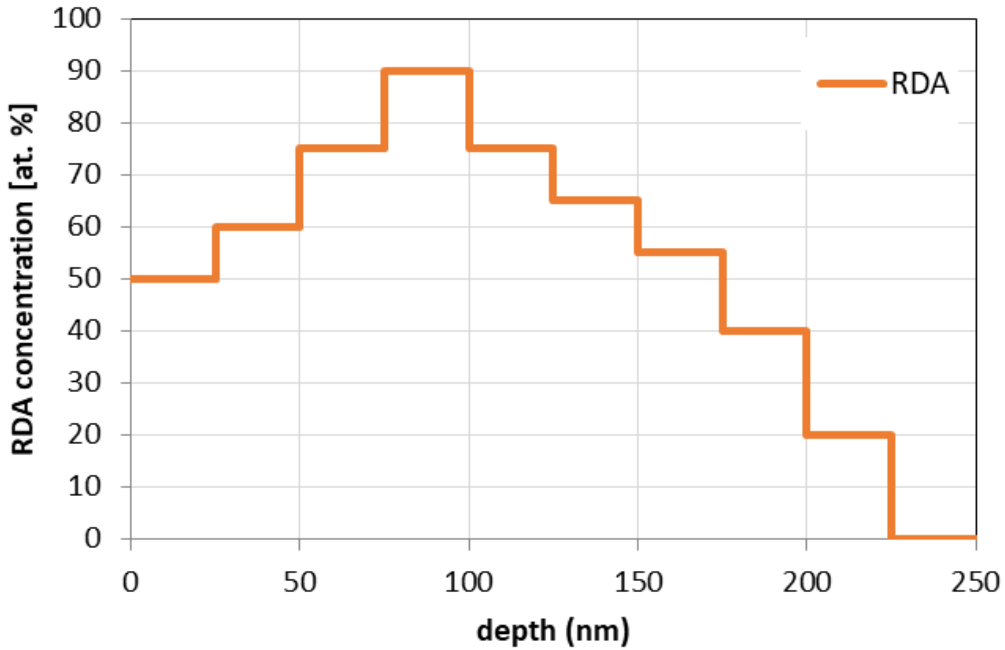


RDA – Randomly Displaced Atoms

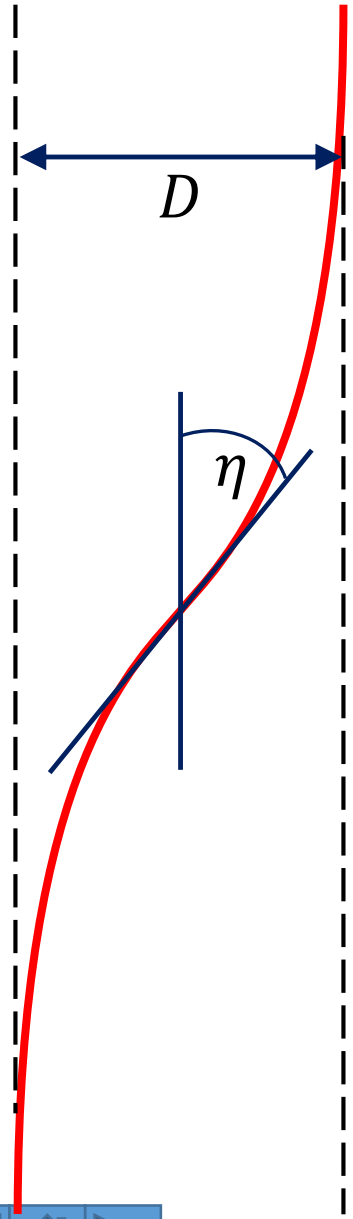
To model one of the most common defect types in crystals, **randomly displaced atoms**, use the **RDA** command. Define a depth distribution of RDA by addressing values of defect concentration at every depth.

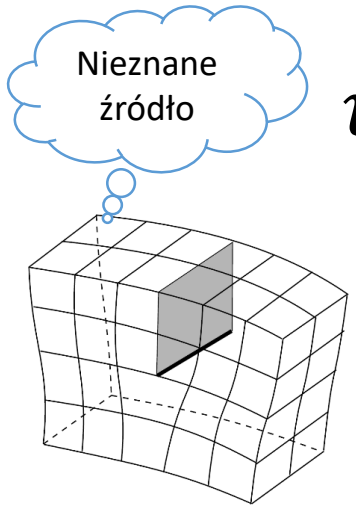


$$f_{RDA} = \frac{N° \; of \; displaced \; atoms}{Total \; N° \; of \; atoms} \; [\%]$$



Model of edge dislocations – DIS





$$u(z) = d \arctan(gz)$$

$$d = \frac{D}{\pi}$$

$$g = \frac{\tan \eta}{d}$$

The model of edge dislocations in McChasy1 is based on the **Peierls-Nabarro** approach. Displacements of atoms due to the presence of a dislocation follow the *arctan* function. Two parameters, *d* and *g*, dependent on a structure and decreasing with the distance from the dislocation, are required.

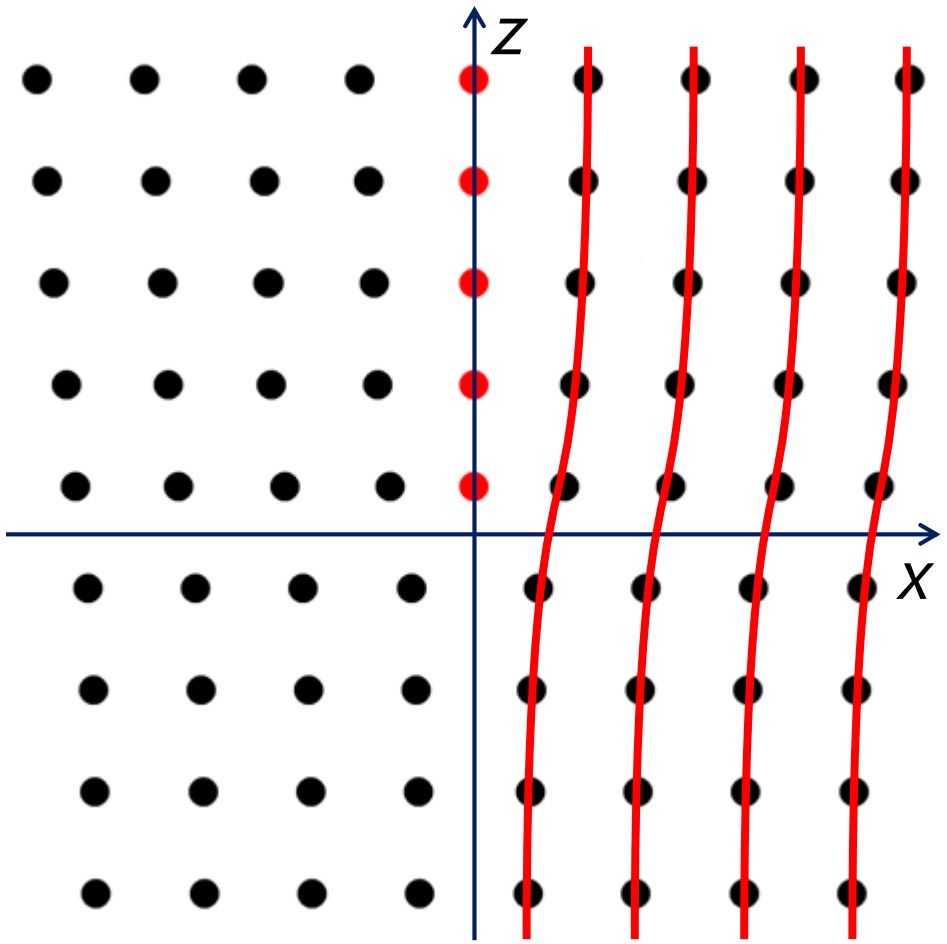
[5] R. Peierls, The size of a dislocation, Proceedings of the Physical Society. 52 (1940) 34–37. https://doi.org/10.1088/0959-5309/52/1/305.

[6] F.R.N. Nabarro, Dislocations in a simple cubic lattice, Proceedings of the Physical Society. 59 (1947) 256–272. https://doi.org/10.1088/0959-5309/59/2/309.

[7] Y. Xiang, H. Wei, P. Ming, W. E, A generalized Peierls-Nabarro model for curved dislocations and core structures of dislocation loops in Al and Cu, Acta Materialia. 56 (2008) 1447–1460. https://doi.org/10.1016/j.actamat.2007.11.033.

[8] P. Jóźwik, N. Sathish, L. Nowicki, J. Jagielski, A. Turos, L. Kovarik, B. Arey, S. Shutthanandan, W. Jiang, J. Dyczewski, A. Barcz, Analysis of Crystal Lattice Deformation by Ion Channeling, Acta Physica Polonica A. 123 (2013) 828–830. https://doi.org/10.12693/APhysPolA.123.828.

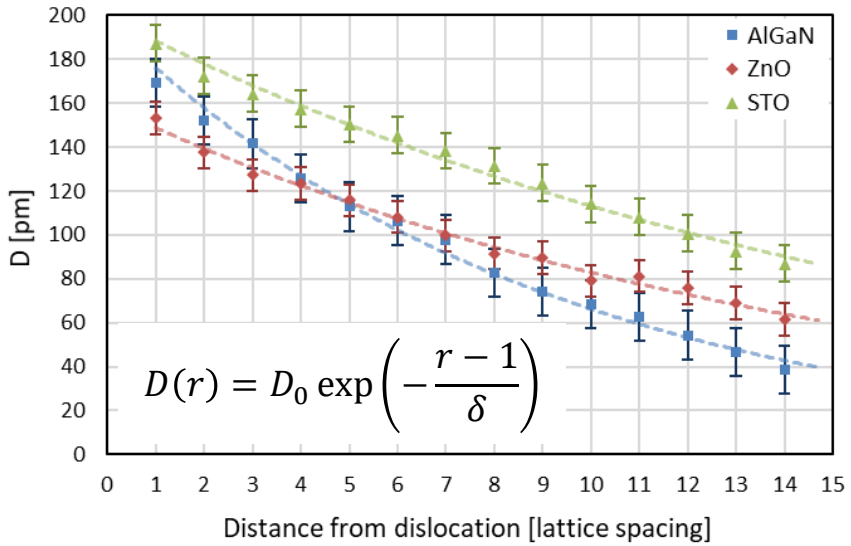
Model of dislocations

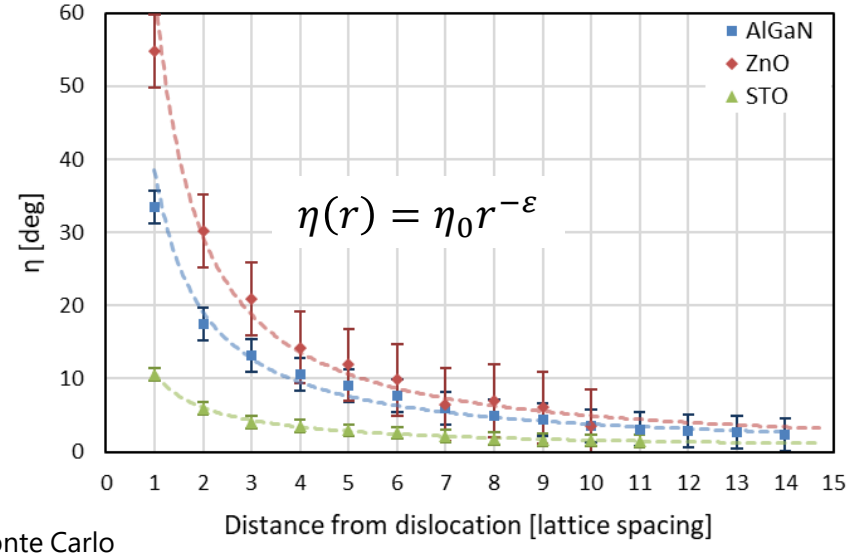


$$D_0 < D_1 < D_2 < D_3 < \cdots$$

$$\eta_0 < \eta_1 < \eta_2 < \eta_3 < \cdots$$

The parameters of dislocations and the character of their decay with the distance from the dislocation have been found using Transmission Electron Microscopy for three structures to date: AlGaN, ZnO, and $SrTiO_3$.





[9] P. Jozwik, L. Nowicki, R. Ratajczak, A. Stonert, C. Mieszczynski, A. Turos, K. Morawiec, K. Lorenz, E. Alves, Monte Carlo simulations of ion channeling in crystals containing dislocations and randomly displaced atoms, Journal of Applied Physics. 126 (2019) 195107. https://doi.org/10.1063/1.5111619.

DIS – Edge DISlocations

rho*weight [x10^{10} cm^{-2}]

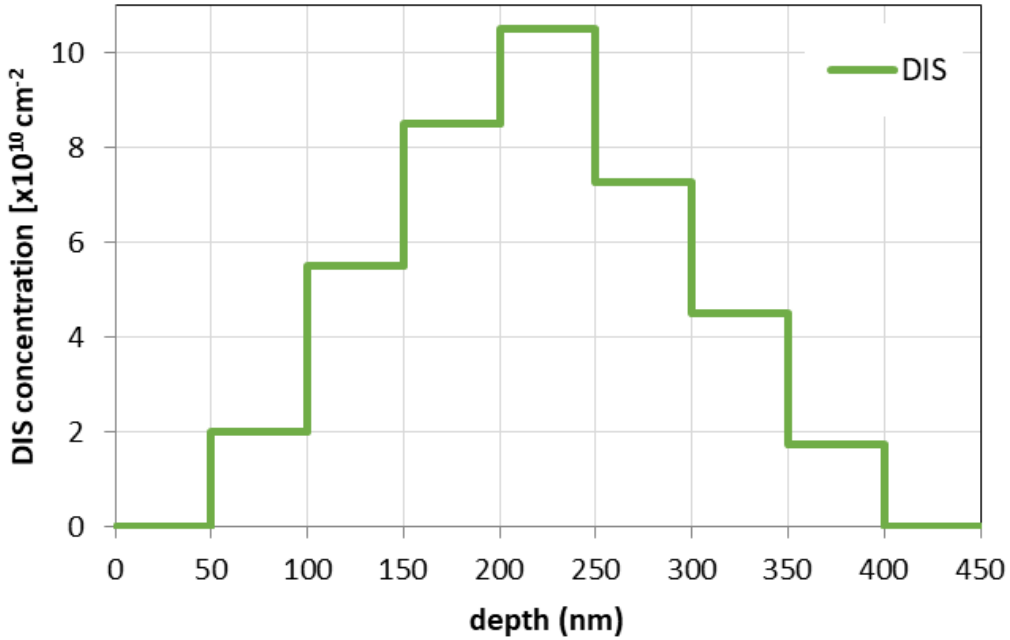
Nº of bent channels

Nº of layers

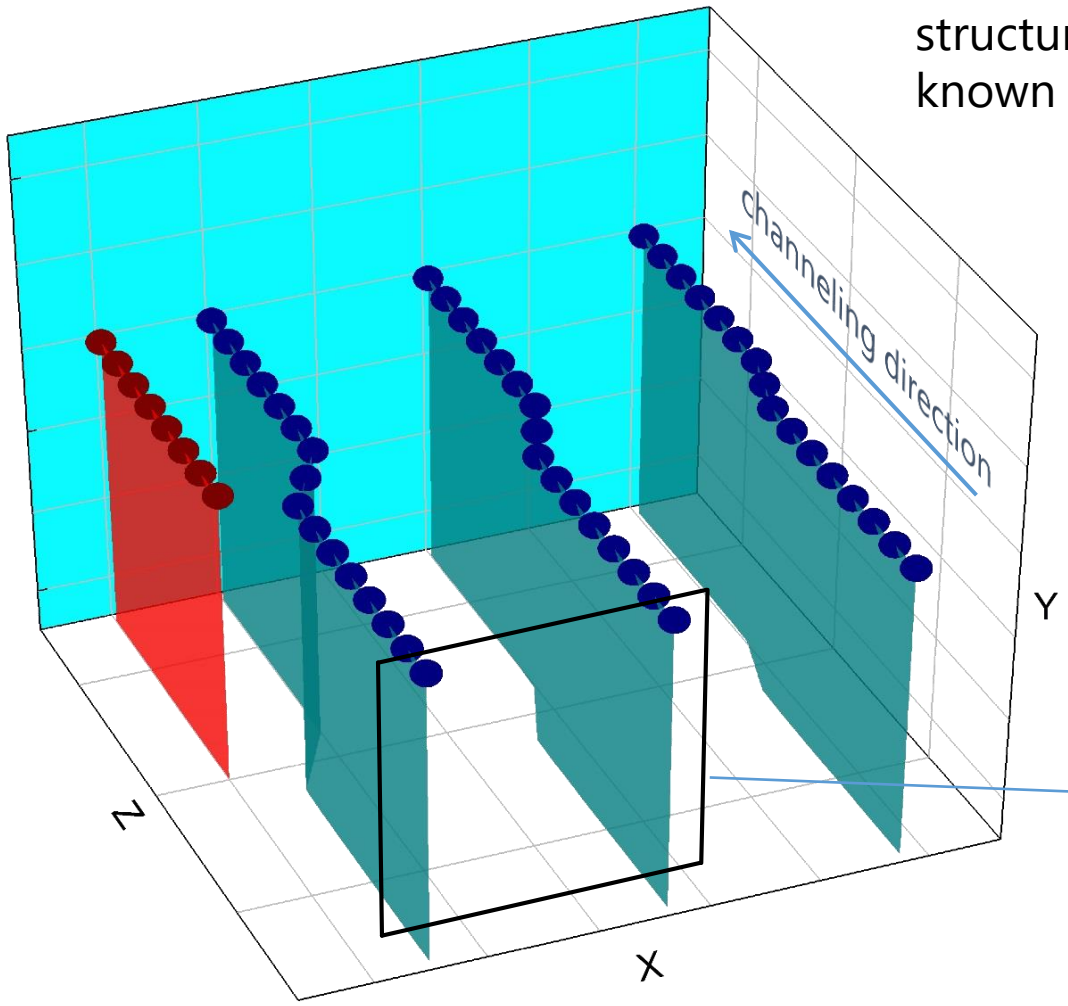
***	rho	n	lay
DIS	1	15	10
***	depth	DISweigh	*DLPweigh*
1	0	0.0	*0.0*
2	50	2.0	*0.0*
3	100	5.5	*0.0*
4	150	8.5	*0.0*
5	200	10.5	*0.0*
6	250	7.25	*0.0*
7	300	4.5	*0.0*
8	350	1.75	*0.0*
9	400	0.0	*0.0*
10	450	0.0	*0.0*

Optional column (see Dislocation loops (DLP)

To define a profile of **dislocations**, use the **DIS** command. Define a depth distribution of DIS by addressing values of defect density at every depth.



Dislocations in McChasy-1



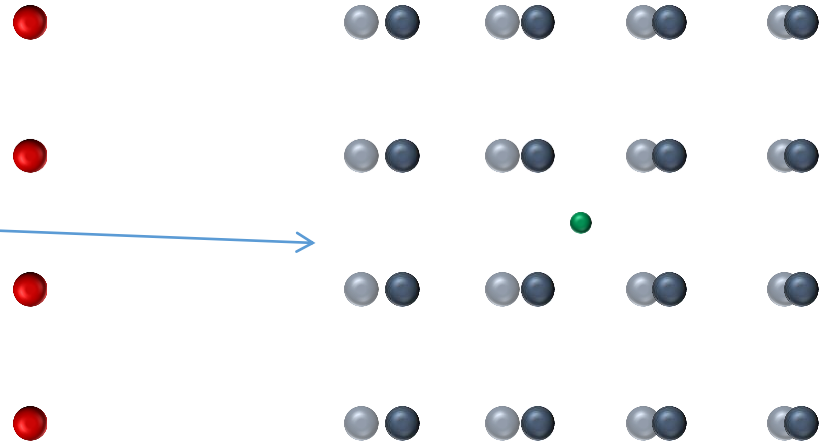
McChasy will displace target atoms using parameters for known structures. A command ATG allows using of parameters of other known structures or defining a new set of parameters.

To use DIS parameters of a selected structure

ATG ZnO

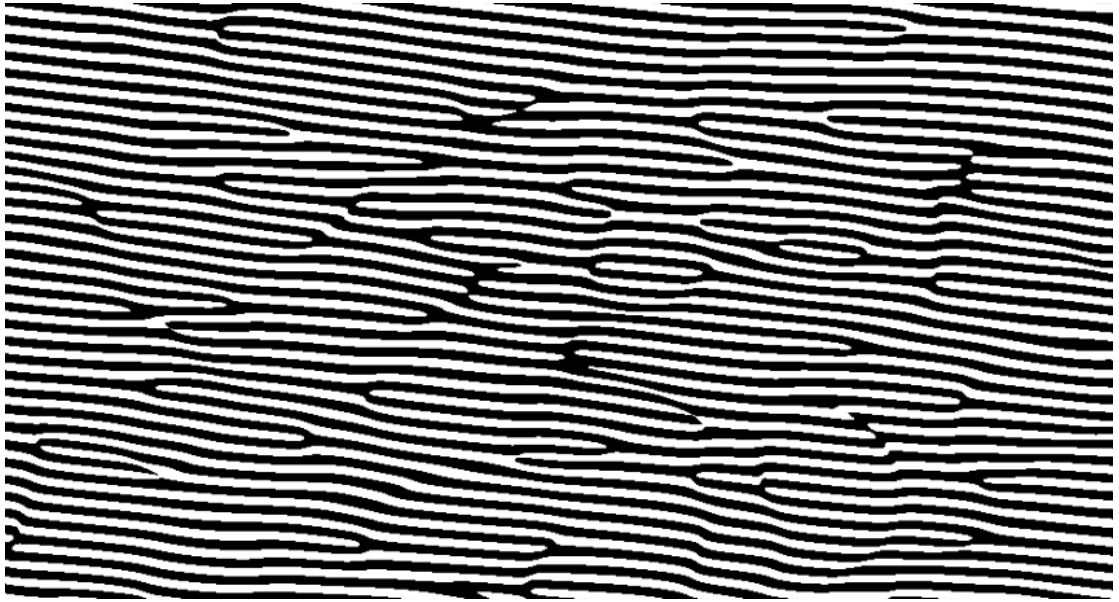
ATG D_0 δ η_0 ε

To use a new set of DIS parameters

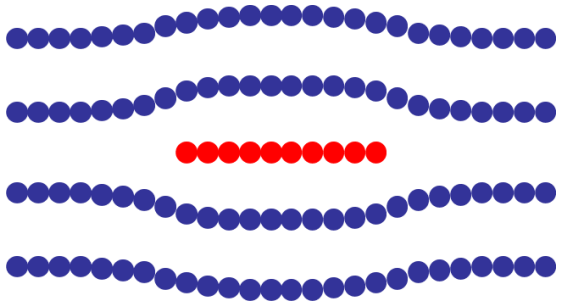


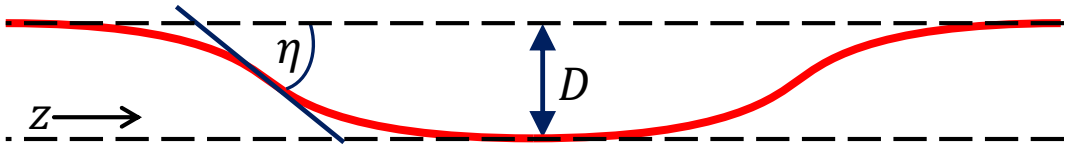
⊗ channeling direction

Dislocation loops



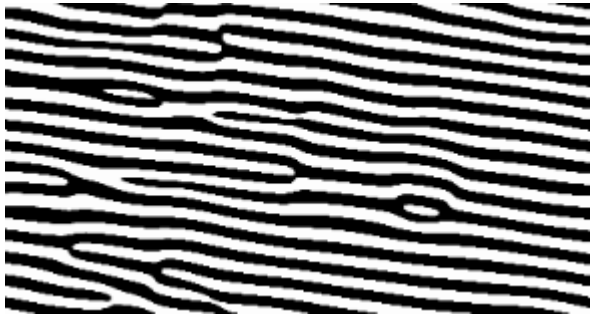
The model of **dislocation loops** extends that of edge dislocations.



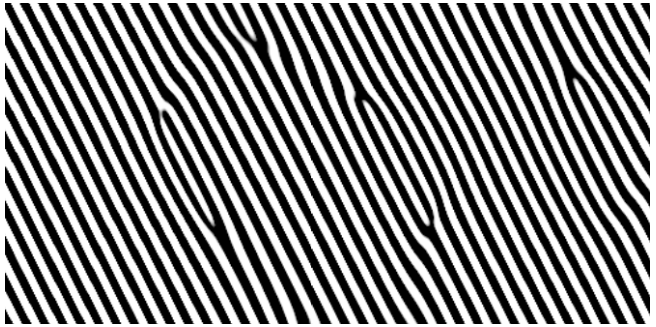


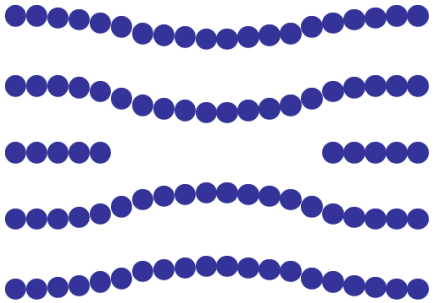
$$u(z) = \frac{D}{\pi}\arctan(gz)$$

Ar-bombarded GaN ↕



Ar-bombarded ZnO ↓





TEM micrographs of ion-bombarded structures

Dislocation loops (DLP)

rho*weight [x10^{10} cm^{-2}]

Nº of bent channels

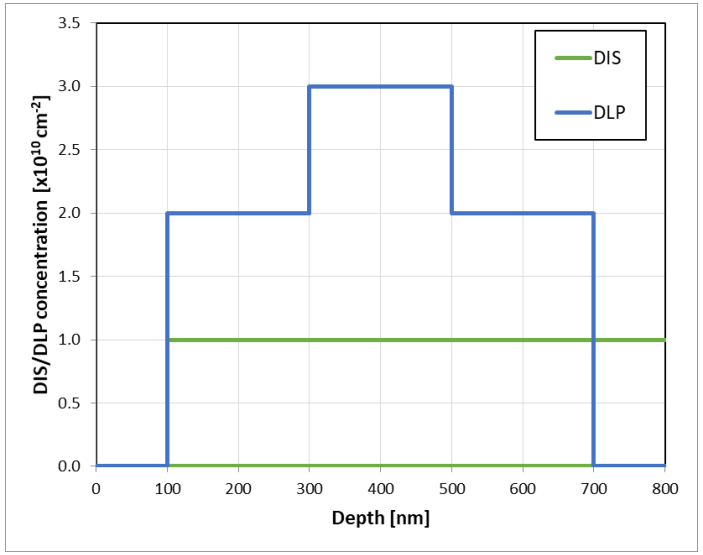
Nº of layers

***	rho	n	lay
DIS	1	15	10
***	depth	weigh	weigh
1	0	0	0
2	100	0.1	0.2
3	300	0.1	0.3
4	500	0.1	0.2
5	700	0.1	0
DLP	10	50	

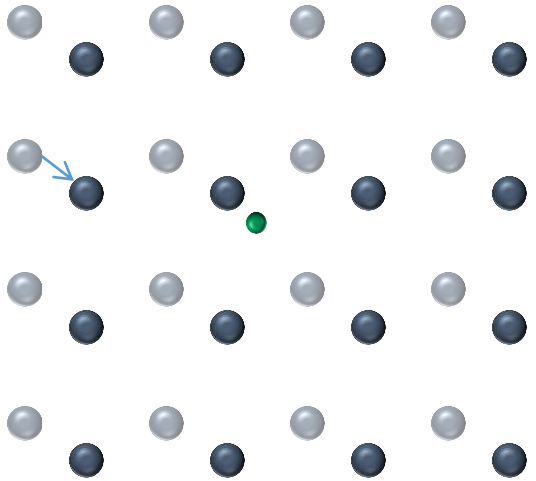
from (DLP size)

to

To define a profile of **dislocation loops**, use the **DIS** command and define a depth distribution of DLPs by addressing values of defect density at every depth in the last column. Use DLP command to define a range of loop sizes.

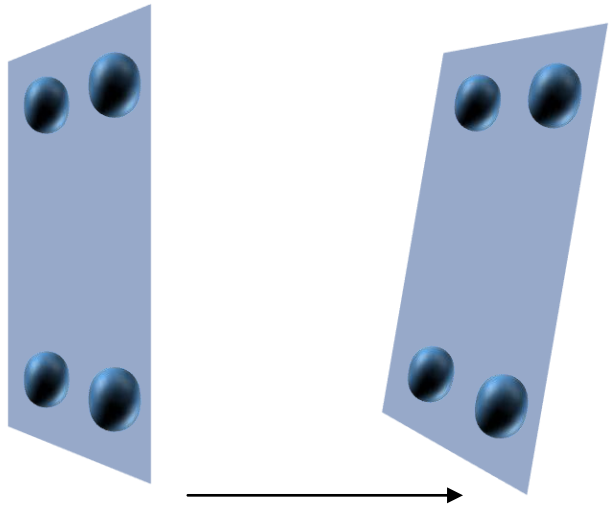


Stacking faults & polygonization



⊗ channeling direction *z*

Other defects avalaible in the **McChasy1** code in a simplified way are **stacking faults (STF)** and **grain boundaries (POL)**. Use with caution (see the Manual for more details).



channeling direction *z*

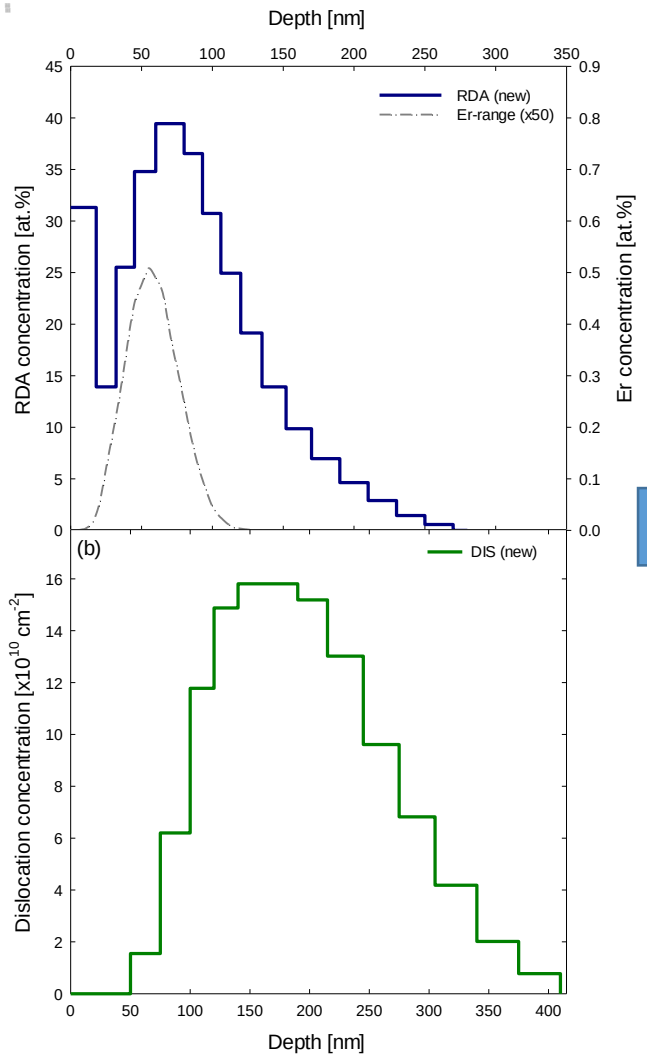
STF	*d*	*x*	*y*
	- *d*istance [nm]		
	- *x* shift [pm]		
	- *y* shift [pm]		

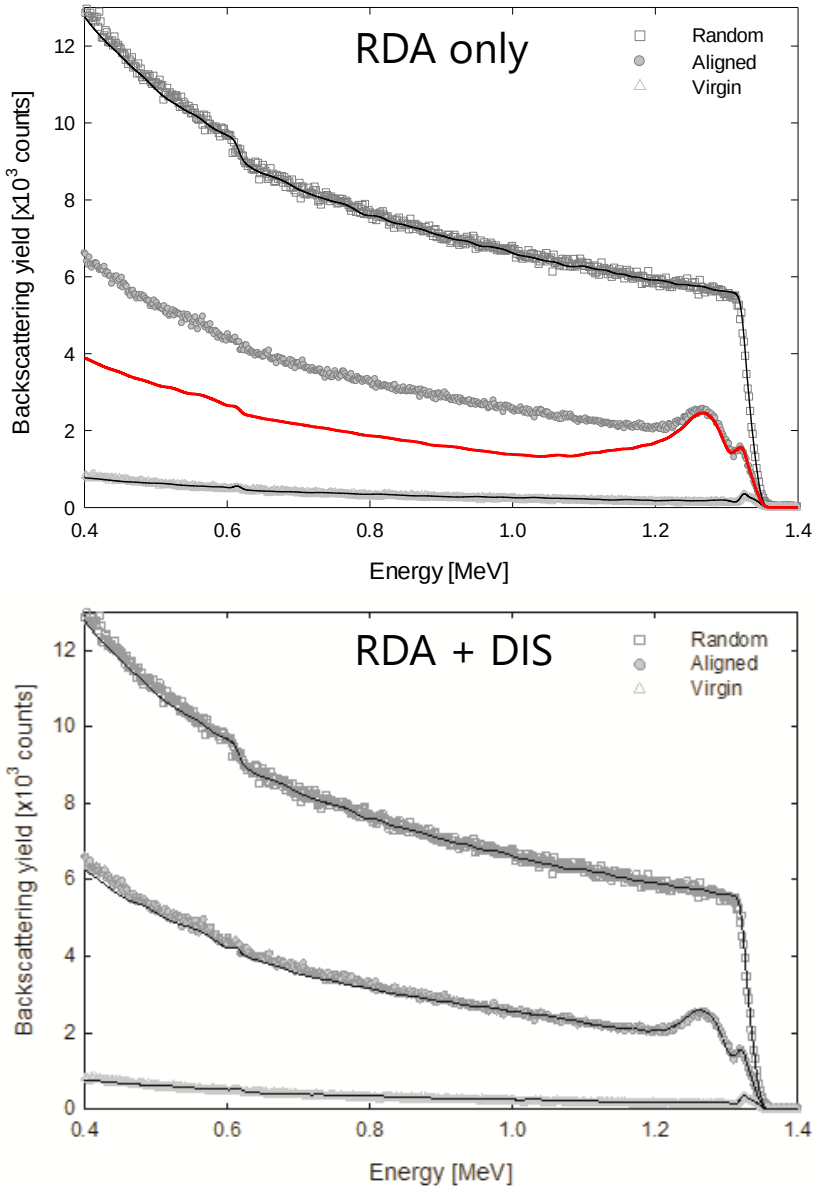
POL	*size*	*shift*	*tilt*	*depth*
	- grain *size* [nm]			
	- *shift* between grains [pm]			
	- *tilt* between grains [deg]			
	- *depth* limit of grain structure [nm]			
example:				
POL	10	150	0.1	300

Example: Er-implanted ZnO

RDA (**R**andomly **D**islpaced **A**toms)

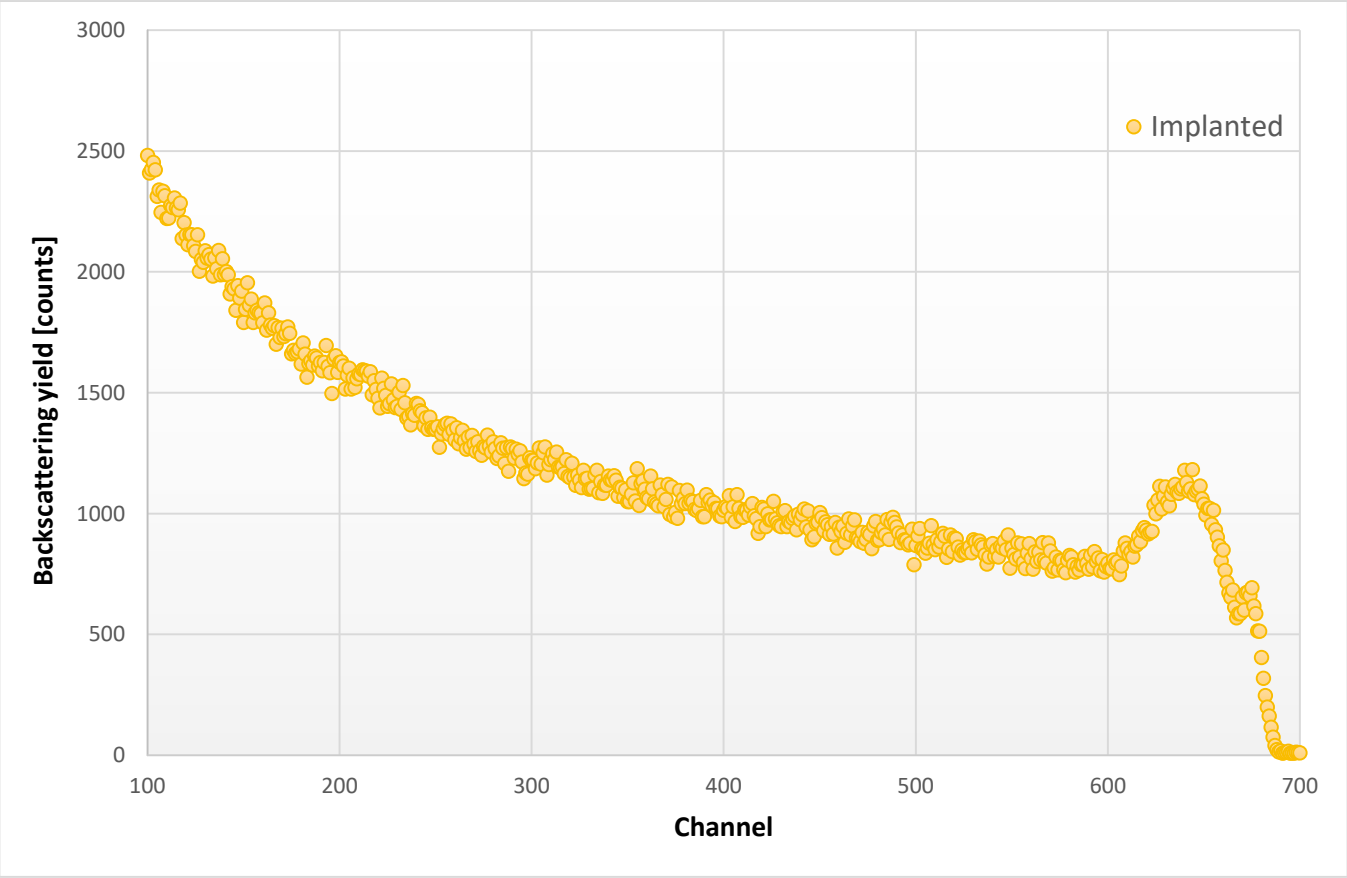
DIS (Edge **dis**locations





A high dechanneling level behind the damage peak in the spectrum recorded for the Er-implanted sample is an indication of **extended defects** created upon ion implantation. A combination of **randomly displaced atoms** and **dislocations** allows the reproduction of experimental spectra correctly and determines defect profiles for both defect types.

Simulations with McChasy



An RBS/C spectrum is a multivariable function, depending on different types of defect. To solve it correctly and unambiguously, one shall consider a system of multiple equations. We will obtain it by measuring the ion channeling spectra at different beam energies and then analyzing them using the **McChasy1** code.

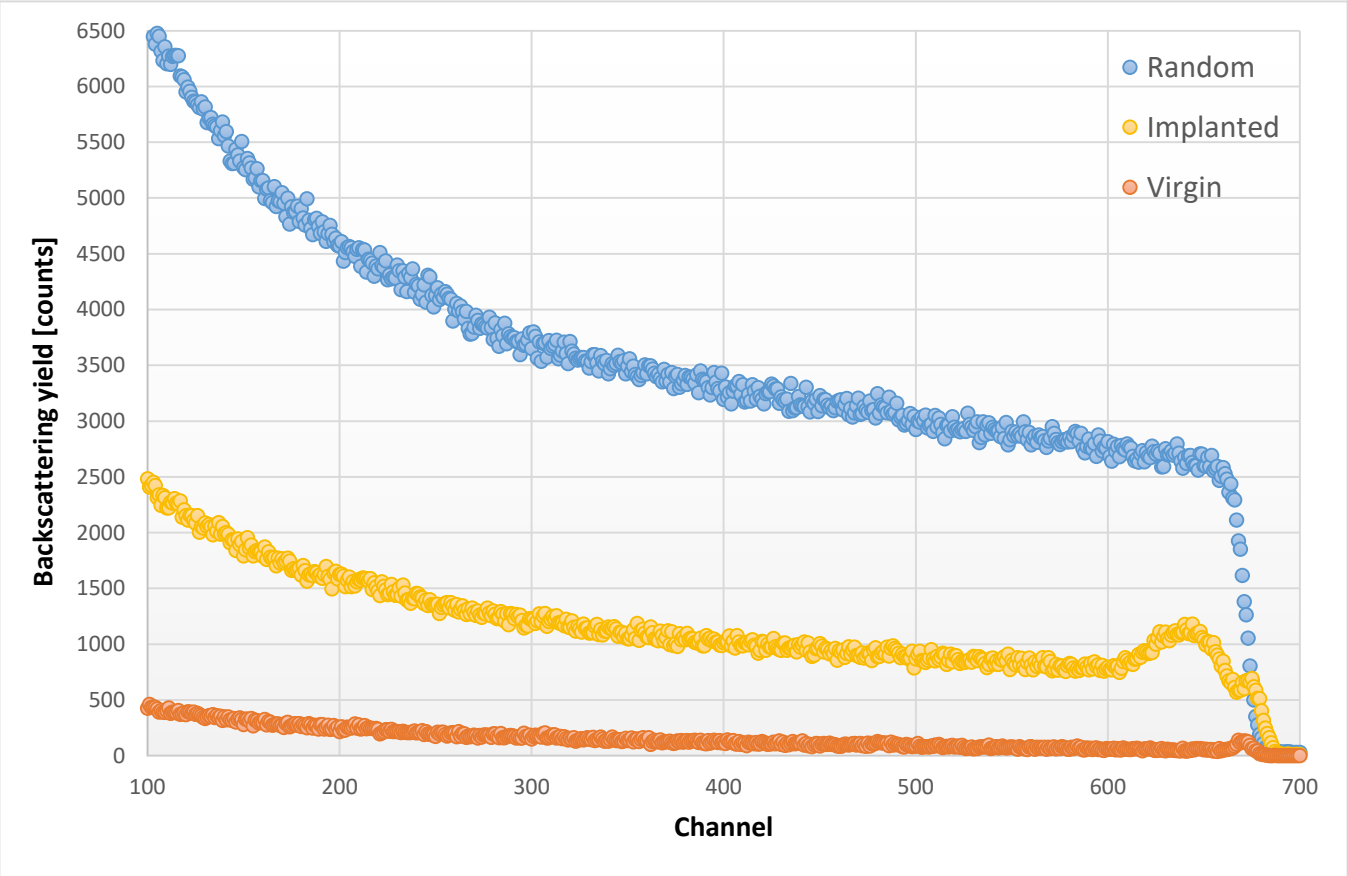
$$y = f(D_1, D_2, \dots)$$

$$\begin{cases} y(E_1) = f(D_1, D_2, \dots) \\ y(E_2) = f(D_1, D_2, \dots) \\ y(E_3) = f(D_1, D_2, \dots) \\ y(E_4) = f(D_1, D_2, \dots) \\ y(E_5) = f(D_1, D_2, \dots) \\ \dots \end{cases}$$

D_1 – RDA
D_2 – DIS
D_3 – SUB
D_4 – STF
D_5 – POL
…

Simulations with McChasy

Typical work with the **McChasy1** code proceeds in three stages. First, a random spectrum should be fitted by adjusting the detector's solid angle and a charge collected during the measurements (**OMC**). Then, thermal vibrations (**VIB**) should be adjusted to reproduce the virgin-aligned spectrum. Eventually, the user should define defect profiles (**RDA**, **DIS**, **DLP**) and compare the simulation results with the experimental spectra until a satisfactory fit is achieved.



Random

- OMC 2.25 20

Virgin (aligned)

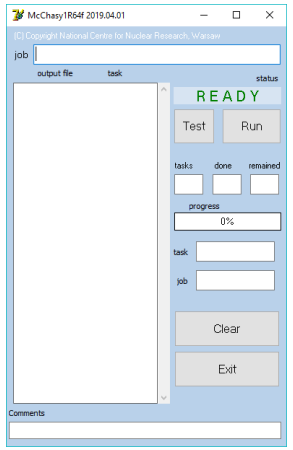
- VIB Zn 10

Implanted (aligned)

- Defect profiles (RDA+DIS)

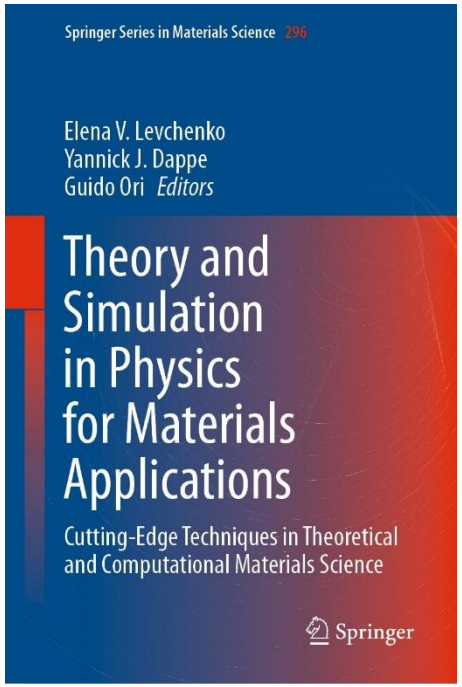
How to cite McChasy?

McChasy-1: the most recent versions containing the model of edge dislocations:



P. Jozwik, L. Nowicki, R. Ratajczak, A. Stonert, C. Mieszczynski, A. Turos, K. Morawiec, K. Lorenz, E. Alves, Monte Carlo simulations of ion channeling in crystals containing dislocations and randomly displaced atoms, Journal of Applied Physics. 126 (2019) 195107. https://doi.org/10.1063/1.5111619.

P. Jozwik, L. Nowicki, R. Ratajczak, C. Mieszczynski, A. Stonert, A. Turos, K. Lorenz, E. Alves, Advanced Monte Carlo Simulations for Ion-Channeling Studies of Complex Defects in Crystals, in: E.V. Levchenko, Y.J. Dappe, G. Ori (Eds.), Theory and Simulation in Physics for Materials Applications: Cutting-Edge Techniques in Theoretical and Computational Materials Science, Springer International Publishing, Cham, 2020: pp. 133–160. https://doi.org/10.1007/978-3-030-37790-8_8.



McChasy-2: the most recent versions:

L. Nowicki, J. Jagielski, C. Mieszczyński, K. Skrobas, P. Jóźwik, O. Dorosh, McChasy2: New Monte Carlo RBS/C simulation code designed for use with large crystalline structures, Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms. 498 (2021) 9–14. https://doi.org/10.1016/j.nimb.2021.04.004.

Past and ongoing projects and collaboration

Ministry of Education and Science

Supporting team

Nuclear Microanalysis Lab,
Plasma/Ion Beam Technology Division (FM2)

- Dr. Renata Ratajczak
- Dr. Kazimierz Skrobas

Nuclear Methods in Solid State Physics Division (FM1)

- Dr. Kamila Stefańska-Skrobas

HZDR
HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

- MIRE (ZnO)

IJCLab Irène Joliot-Curie Laboratoire de Physique des 2 Infinis

✓ Dr. Frederico Garrido

- STIRI/COPIN

ipfn INSTITUTO DE PLASMAS E FUSÃO NUCLEAR

✓ Dr. Katharina Lorenz
✓ Dr. Eduardo Alves

- NASIB (GaN, InGaN, SHIs)
- RaDeNiS (Ni & Ni alloys)
- DiGaN (GaN: N-, Ga-polar)