Channelling Theory and Simulation

- Channelling Applications
- **The FLUX Code**

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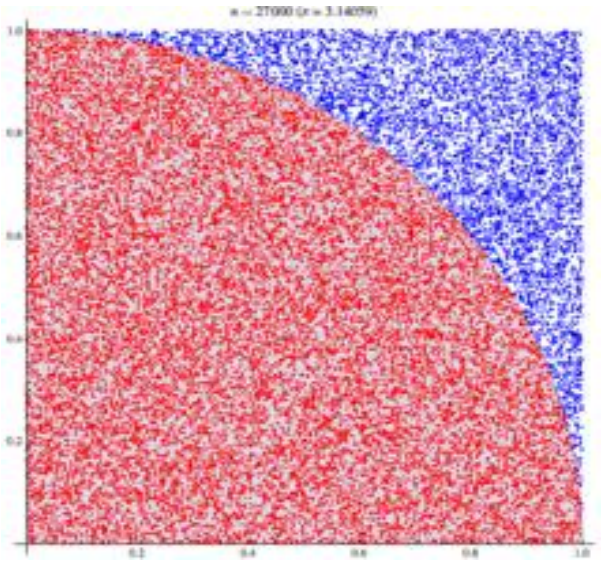
Outline

- **Introduction:**
- Monte Carlo Simulations

- **The FLUX Code**
- The Principle
- Main Input Files
- Examples

Monte Carlo method



Computational algorithm that relies on repeated random sampling to obtain numerical results.

Example: Determination of π: The ratio of the areas of the quarter circle and the square is π/4

1. Draw a square and then inscribe a circle within it (definition of possible domains)
2. Uniformly scatter some objects of uniform size (grains of rice or sand) over the square (generation of random input parameters)
3. Count the number of objects inside the circle and the total number of objects (analysis of input data)
4. The ratio of the two counts is an estimate of the ratio of the two areas, which is π/4. Multiply the result by 4 to estimate π (numerical result)

Monte Carlo for Scattering Events

- The ideal technique since scattering events themselves are of statistical nature (collisions and random thermal vibrations).

- Input parameter are chosen in a random way based on average probabilities:

  - Entrance point at surface (position in unit cell) and impact parameter
  - Thermal vibration amplitude of matrix atoms
  - Angular divergence of the particle beam
  - Azimuthal angle after collision

Monte Carlo/channelling

- The occurrence of the channelling effect was first recognised using the MC code Marlowe [APL 2 (1963) 30]

  (although channelling was first predicted by Stark in 1912; Phys. Zeitschr. XIII, p. 973):

THE CHANNELING OF ENERGETIC ATOMS IN CRYSTAL LATTICES

Mark T. Robinson and O. S. Oen

Solid State Division, Oak Ridge National Laboratory[1]

Oak Ridge, Tennessee

(Received 5 December 1962)

The recent development of sophisticated experimental techniques, particularly by J. A. Davies and his coworkers,[2,3] has led to the accumulation of a considerable amount of information on the penetration of ions of moderate energy (1 to 100 keV) into solids. Previous theoretical studies of the problem[4–6] have been restricted by the assumption that the atoms of the solid were randomly located in particles stopped in the target, the half-thickness of the tail increasing with the energy of the bombarding ions.

Our recently reported computer studies of the slowing down of atoms in solids[5,6] have now been extended to a model in which the atoms are correctly located on lattice sites. The moving particle loses its energy in binary elastic collisions with

- "These "channelled" particles …experienced very many glancing collisions with atoms of the lattice…"

Channeling Simulations

- Several codes were developed in the 1970s based on analytical approaches following Lindhard's theory of channelling. (continuum string approximation assuming the conservation of transverse energy – not correct due to multiple scattering with nuclei and electrons)

- First MC program LAROSE was developed by Barrett at [J.H. Barrett, Phys. Rev. B 3 (1971) 1527]

- FLUX was developed in the 1980s by Peter Smulders and Dik Boerma and is, since then, freely available to the community. [NIMB 29 (1987) 471].

The FLUX Code

NIMB 29 (1987) 471

COMPUTER SIMULATION OF CHANNELING IN SINGLE CRYSTALS

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Received 25 November 1986 and in revised form 7 September 1987

A Monte Carlo program for the calculation of channeling phenomena is described. The program combines the binary collision model and the multistring approximation. The energy loss due to electronic excitation is taken into account, with the use of the model of Dettmann and Robinson for the inner-shell electrons and the theory of Pines for valence electrons.

The output of the Monte Carlo program may be used for the determination of the impurity sites in single crystals, via a set of auxiliary programs, that enable that calculation of the impurity yield and the analysis of experimental channeling dips. As an application, the site determination of iodine in silicon is described.

Another application is the simulation of RBS spectra of planar channeling ions. Simulated and experimental spectra are compared for 1 MeV ions in the (110), (111) and (100) planes of silicon. A reasonable agreement was found. The possible causes of the remaining deviations are discussed.

- Download at: http://www.pjms.nl/flux.html/
- The file distribution contains a lot of useful documentation and secondary programs as well as a presentation given by Peter Smulders in Lisbon in 2004.

What is FLUX?

- The distribution contains several programs and subroutines being the one called “FLUX” the main tool.
- FLUX is a code based on MC that follows the trajectories of ions entering the crystal at an angle θ ($\theta < 15^{o}$) with a major crystal axis.

$\rightarrow$ Main output:

- Flux distribution within the channel
- The close encounter probability as a function of depth
- Average energy loss and energy straggling

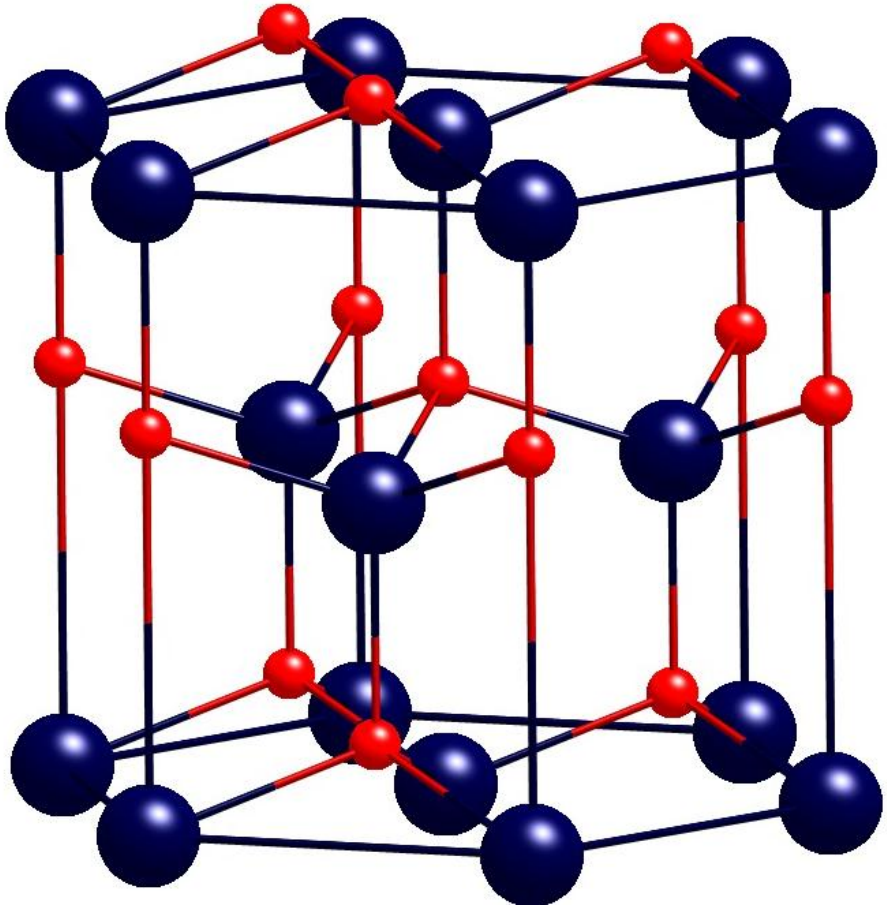
- Complementary programs in the package:
  - Preparation of input files (i.e. calculation of energy loss)
  - Analysis of output files (i.e. simulation of RBS spectra, calculation of impurity yields for lattice site location measurements)

The Principle

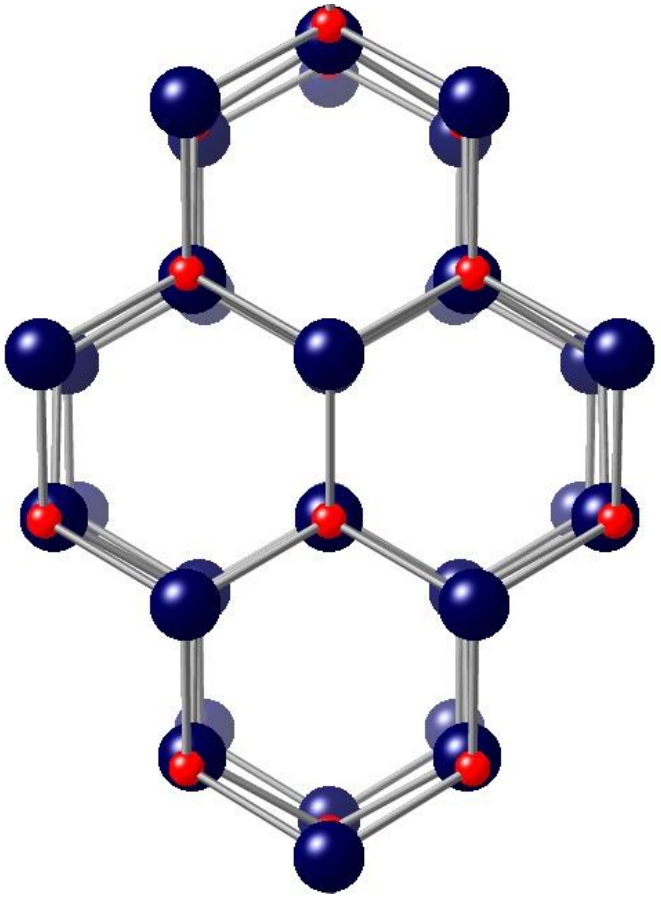
1. The motion of the ions is treated classically (valid for protons and heavier particles).
2. The starting points of trajectories are generally selected at random over the surface of the crystal.
3. Thermal vibrations are simulated by giving each lattice atom a random displacement assuming Gaussian distribution following Debye's theory.
4. Collision events are described by an adequate potential: binary collisions or continuum string model.

Wurtzite GaN Crystal

Wurtzite GaN lattice



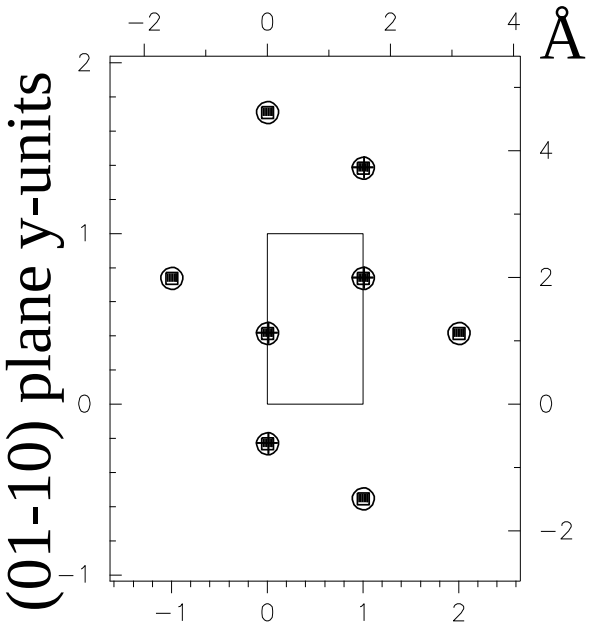
Projection along the c-axis



Definition of the crystal axes: GaN

Projections along different channelling directions

<0001>



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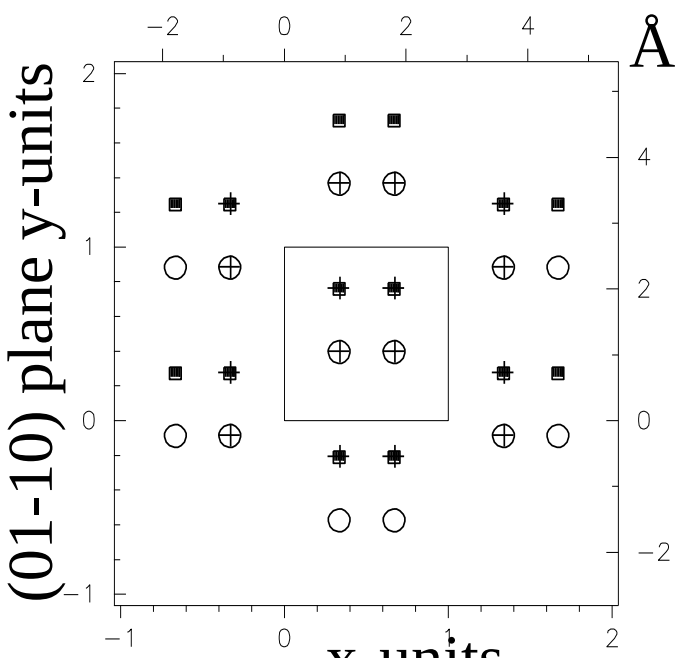

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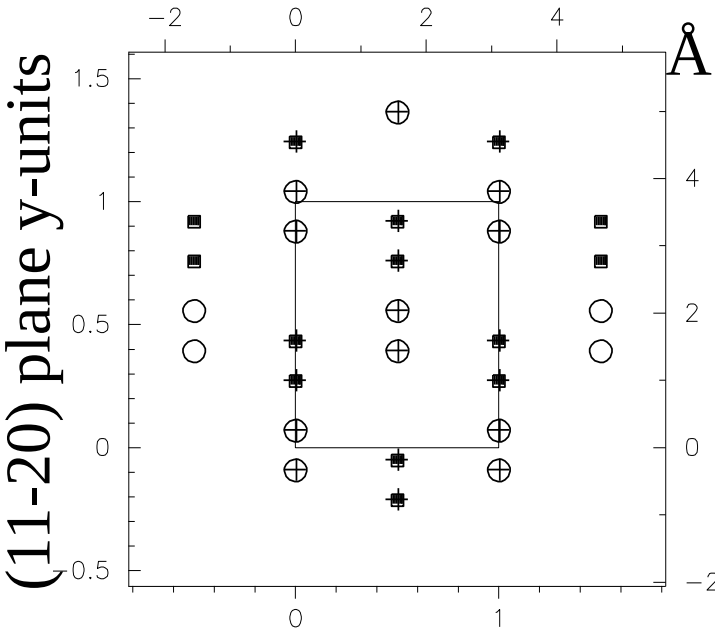


- A unit cell is defined which by simple symmetry transformations describes the entire lattice (combin.fig; combi4.fig).
- If an ion leaves the unit cell it will be put back into the unit cell in an equivalent position: translation of the coordinates of the ion and/or a reflection of its velocity components (symmetry transformations in symmetry.inc and yimp)

Binary Collision Model

- Atomic rows inside and close to the unit cell (distance < ~2 Å) will be treated using binary collisions (outer rows will be treated in the continuum string approximation).

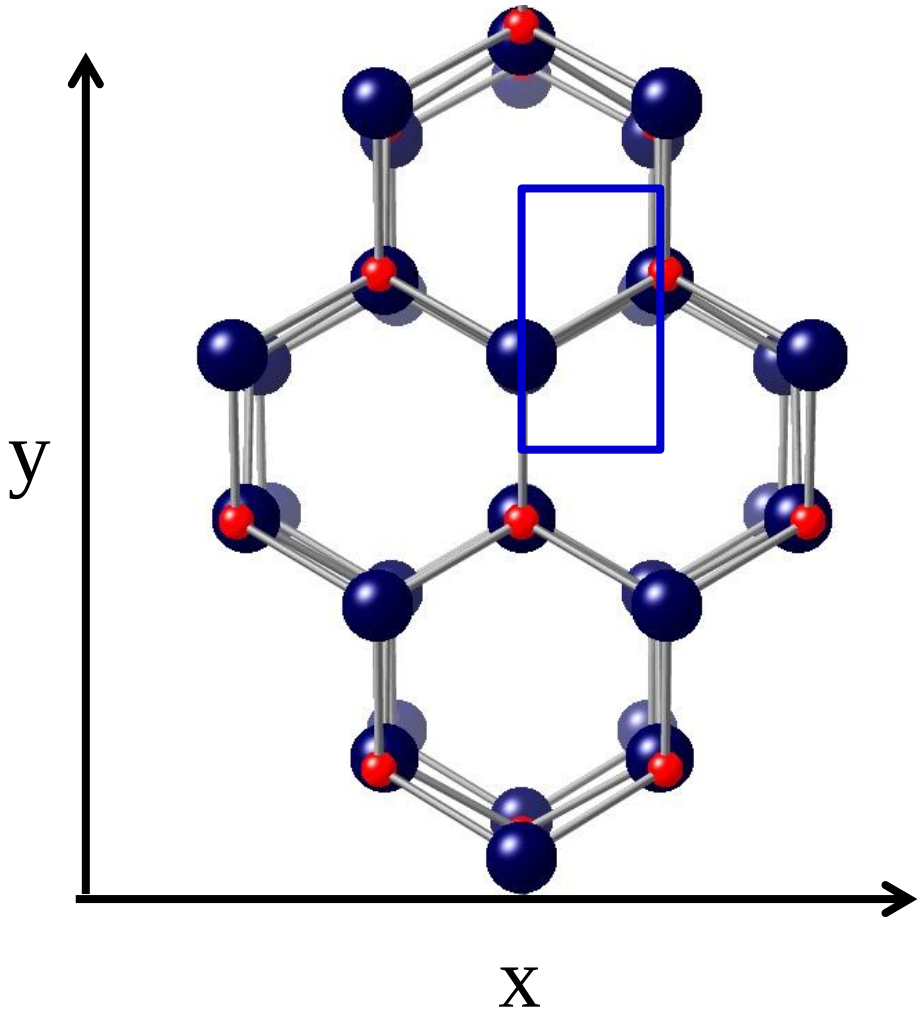
- Passage of ion in matter is treated as a sequence of independent binary collisions between the probing ion and the matrix atoms.

- The collision causes a change in the linear momentum vector.

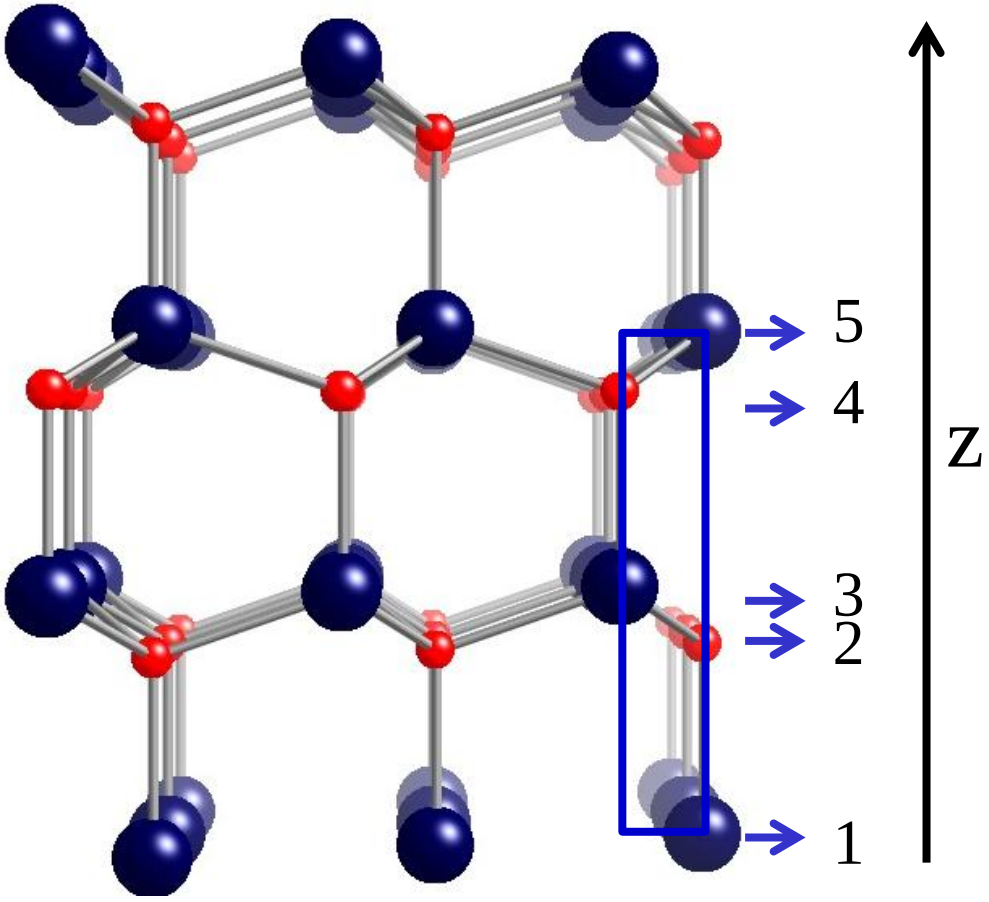
- The linear momentum is re-evaluated at each atomic plane perpendicular to the channelling direction.

GaN Wurtzite Crystal

Projection along the c-axis



Projection along the a-axis



→ Update of linear momentum vector at each plane (1-5)

Binary Collision Model

- Collisions take place at certain depths at each encountered atomic plane.
- Between planes the particles travel in straight lines.
- The particle position and velocity are up-dated taking into account:

  - a binary collision with the atoms (of the rows marked for binary collision)

  - the deflection due to surrounding strings (of the rows marked for continuum string)

  - the energy loss and angular scattering due to interaction with electrons

- The force causing the change in transverse linear momentum $\Delta p = \int F_{\perp} dt$ is defined by an appropriate potential.

Interatomic Interaction Potentials

Screened Coulomb Potential:

$$V(r) = \frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0 r}\varphi(r, Z_1, Z_2, E)$$

properties of screening function φ:

- for r << atomic radii (ratio of radii of atom and nucleus ≈ 10^4)

  small influence of electrons → $\varphi(0, Z_1, Z_2, E) = 1$

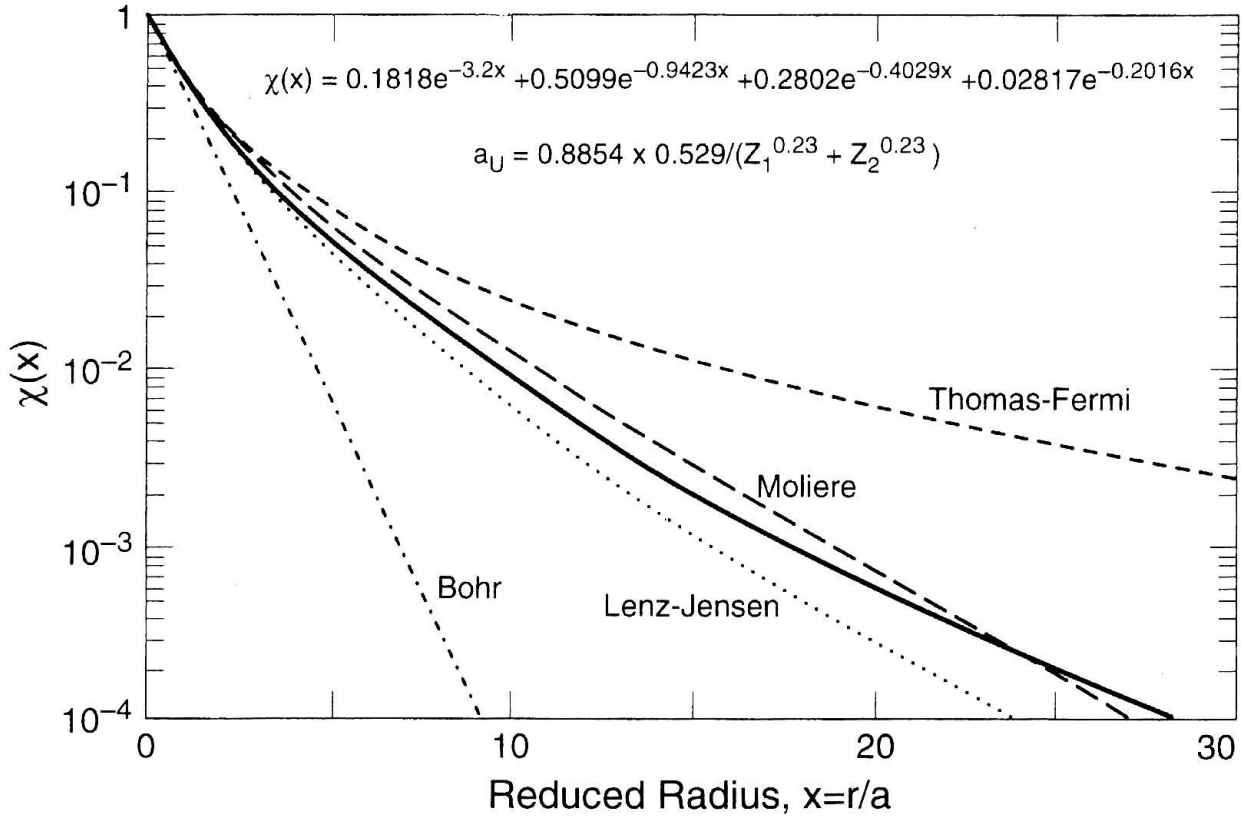
- for increasing r

  increasing screening due to electrons, decreasing screening function

- for r >> atomic radii

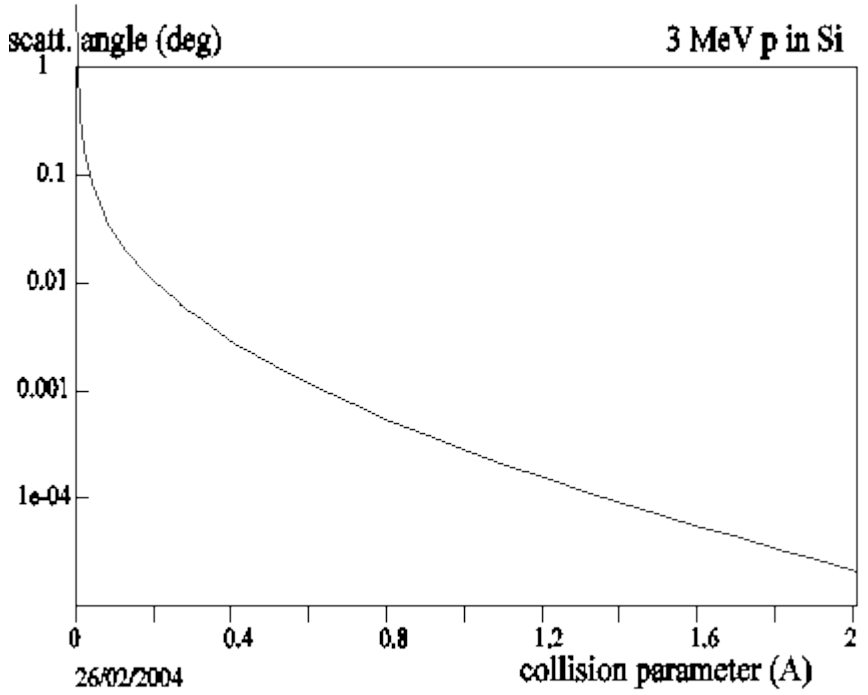
  complete screening → $\varphi(0, Z_1, Z_2, E) = 0$

Different Screening Functions



In FLUX one can choose between Molière, ZBL (universal), Hartree-Fock
→ For most applications the differences are negligible (on the other hand e.g. flux peaking is strongly dependent on the potential)

Scattering angle as a function of impact parameter



→ The interaction takes place mainly in the direct vicinity of the nucleus, for an impact parameter of 2 Å the scattering angle is in the order of 10^{-5o}. (therefore the rule of thumb to treat rows with less than 2 Å distance with binary collisions)

Energy loss and thermal vibrations

- **Nuclear energy loss** is of course automatically taken care of by the binary collision model

- **Electronic energy loss** is taken into account by two components:
  - impact parameter dependent inner electron shells
  - interactions with outer shell electrons, assumed to be uniformly distributed (not necessarily the case e.g. strongly directional covalent or ionic bonds)

  (models are probably out-dated and could be improved)

- **Thermal vibrations** are accounted for by random sampling the position of the atom from a Gaussian distribution at each collision event. (correlations in the vibrations of adjacent atoms are neglected)

FLUX Output

The output-file (name.flx or name.fla) contains:

- the close encounter probability as functions of depth,
- the energy loss (z),
- the energy straggling (z),
- flux distribution integrated over depth as a function of x and y.

Andrés' installation guide for Windows

FLUX 7.9.1 INSTALLATION FOR WINDOWS7 (32 or 64 BITS) (tested also in Windows 8)

#uses parallel processing on multiple-CPU systems
#is compatible with the gfortran compiler (but also with g77)

1. Install MinGW
Download MinGW program mingw-get-inst-20120426.exe
Install it in C:/MinGW as suggested
Install everything, including the MSYS and the Dev. Toolkit
Be sure all the files were downloaded at 100% (no errors)

2. Install GrWin
Download the GrWin program GrWinC-100e_MinGW_gfortran.msi
Install it in C:/GrWin
Make the complete installation

3. Run msys.bat in C:/MinGW/msys/1.0/
Running msys the program will automatically create a folder for the USER in /home.
Close the command line (exit).

4. .profile

This is a very important file that is not install with the MinGW, defining the paths for FLUX and GrWin.
Copy or make a file .profile in C:/MinGW/msys/1.0/home/user
The lines for the file are:

```
PGPLOT_DIR=/c/GrWin/
export PGPLOT_DIR
PGPLOT_DEV=/GW
export PGPLOT_DEV
FLUX=$HOME/flux7.9.1/FLUX7
export FLUX
PATH=.:${FLUX}/BIN:${PATH}
TERM=msys
export TERM
LESSCHARSET="iso8859"
export LESSCHARSET
```

Run msys.bat again to apply the changes in .profile and close it.

5. Install FLUX7
Copy the flux7.9.1.tar.bz2 in C:/MinGW/msys/1.0/home/user
Run msys.bat

```
> tar -jxvf flux7.9.1.tar.bz2
```

This will create the folder /flux7.9.1/FLUX7

```
> cd flux7.9.1/FLUX7
> makemake          (list of programs to compile)
> make clean        (clean previous compilations)
> make              (compile FLUX)
```

6. Final tests

```
> testall
```

This executes a set of tests for flux and it should give several graphical windows.

1. Planar channeling phase maps at different depths (5 graphs)
2. Lattice GAAS211 and LINEOC017 (2 graphs)
3. Tracks in Mo (bcc) lattice (4 graphs)
4. Tracks in GaAs and bent crystal (2 graphs)
5. RBSsim (3 graphs)
6. FitYim (2 graphs)

```
> cd INPUT
> fluxvelo.bat
```

This executes a job to test the speed.
8-core computer: record in 135 s
4-core computer: about 253 s.

7. To execute FLUX:

```
> makeflx test.inp
```

Input file for <0001> GaN

NLAYER 1	Number of layers (1 or 2 is possible)
LATTICE WURTZ0001	Identifier for lattice type and projection
2	nº of constituents (Ga+N)
2 31 7 4.0026 70 14	Atomic number and mass number of He, Ga, N
-0.07, -0.07	Vibration amplitude for Ga and N (or Debye temperature)
293	temperature
3.19 5.19	a and c lattice parameter
XYOUT 10	Flag to output x-y coordinates needed e.g. to plot the ion tracks

Input file for <0001> GaN

```
T0
2.0 0.1
```

→ Initial energy of channelling particle and minimum energy after which ion is no longer followed

```
DEDX WEIGHTED
```

→ Used if RBS spectra are to be simulated
Energy loss of backscattered particles is larger than the average

```
DEDX VALENCE
5.9771    7.6763
```

→ Energy loss in eV/Å for valence electrons
Localised electrons/plasma electrons
→ Calculated using the program DEDX
Model by Melvin and Tombrello Rad. Eff. 26(1975) 113.

Input file for <0001> GaN

ELCORE

2432.52719 1394.16791 927.
482.28758 405.36406 342.(
212.45975 184.11106 160.9
113.40961 102.45768 93.1
71.87355 66.35234 61.38
49.02208 45.56145 42.36
34.13424 31.77630 29.59
23.89644 22.26473 20.74
16.79307 15.65777 14.60
11.86506 11.08075 10.34313 9.66561 9.03278
424.72090 299.60550 197.75180 129.86430 89.04152
65.89589 53.11787 46.01823 41.88944 39.26606
37.39231 35.88521 34.56129 33.33233 32.15735
……..

Energy loss in eV/Å due to core electrons: 50 values for different impact parameters (up to 2Å) and for each element

Values generated with the program DETTMANN. Input to this program are the electron binding energies for the various shells.

Model by Dettmann and Robinson: PRB 10 (1974) 1

Input file for <0001> GaN

```
ZDIST UNIFORM
    1500
```

→ Maximum depth in Å
Uniform impurity distribution

```
FLUX
100
```

→ Flag asking for output of the ion flux

```
NBIN
83
```

→ nº of bins to use in distribution of nuclear encounter probability, energy loss etc. with depth

```
CROSS SECTION
-1
-1
-1
```

→ Rutherford cross section

Input file for <0001> GaN

```
BEAM DIVERGENCE
0.08      0.08      0
```

→ Beam divergence: horizontal and vertical standard deviation

```
NTRACKS
100
```

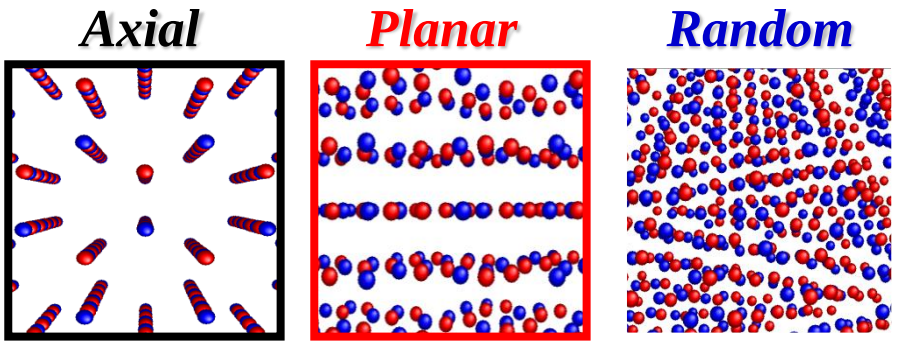
→ nº of tracks (in this case only few in order to plot the track distributions)

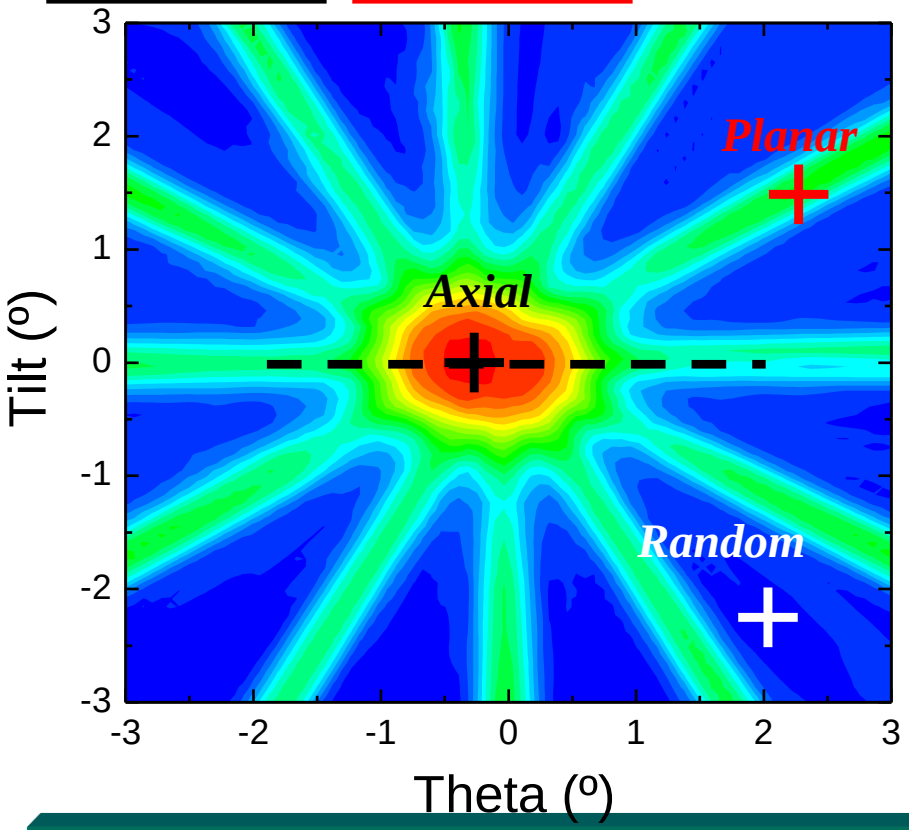
```
ANGLES
1
0 0
```

→ nº of incidence angles (here just one but one can list all angles of an angular scan here or even 2D maps)

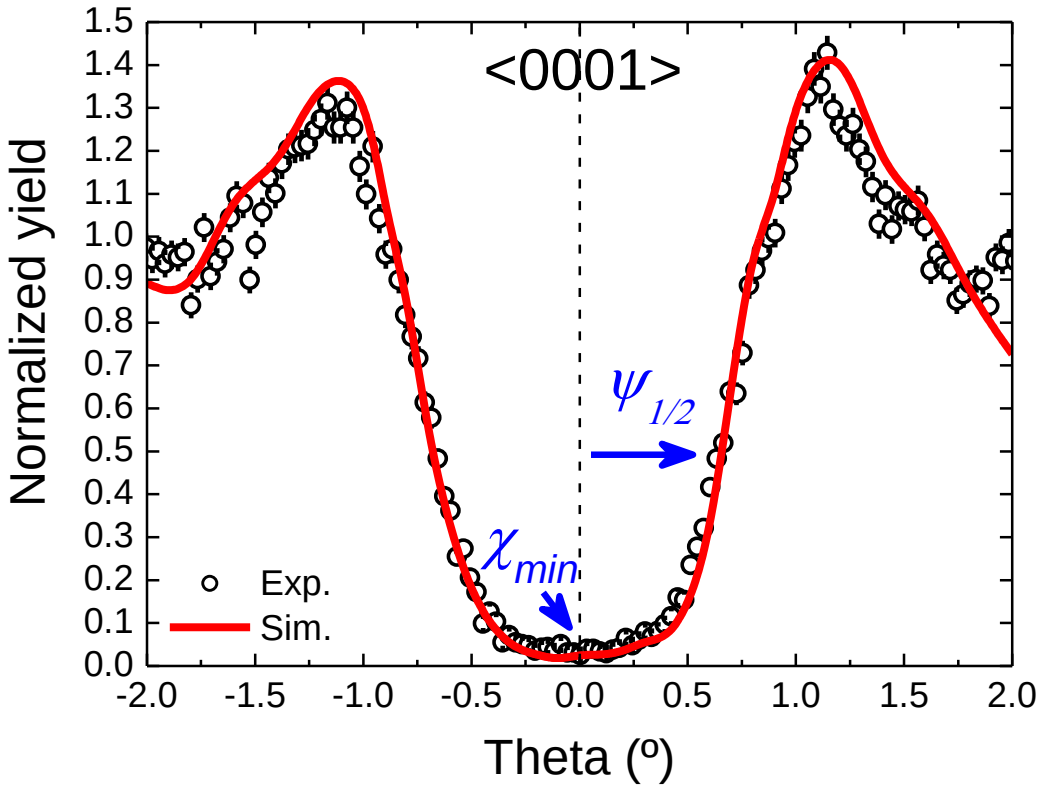
1st number: tilt with channelling direction
2nd number: angle with x-axis of unit cell (defines the channelling plane)

FLUX simulations in GaN





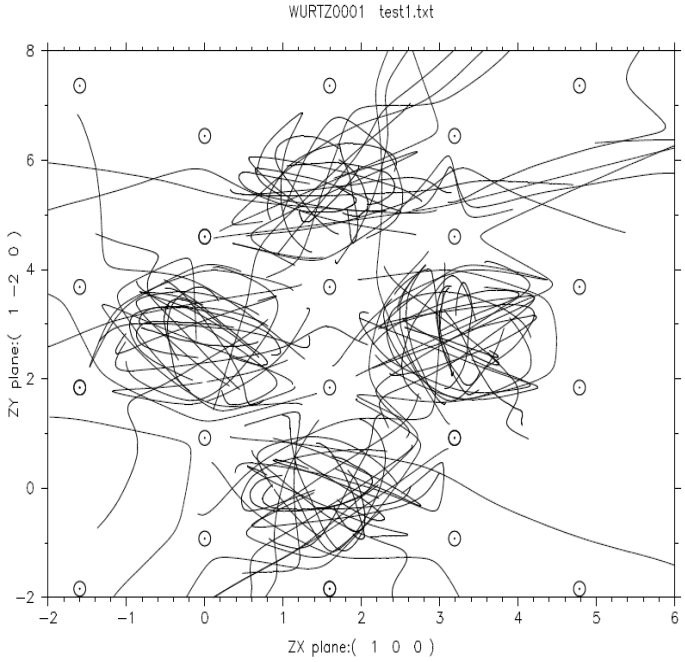
Linear scan across <0001> in GaN

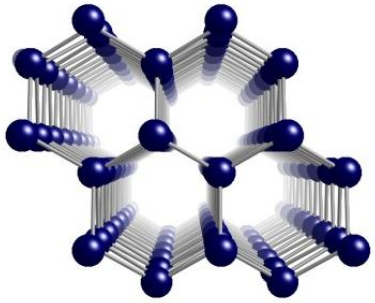


⇒ Excellent agreement of experimental data and simulation

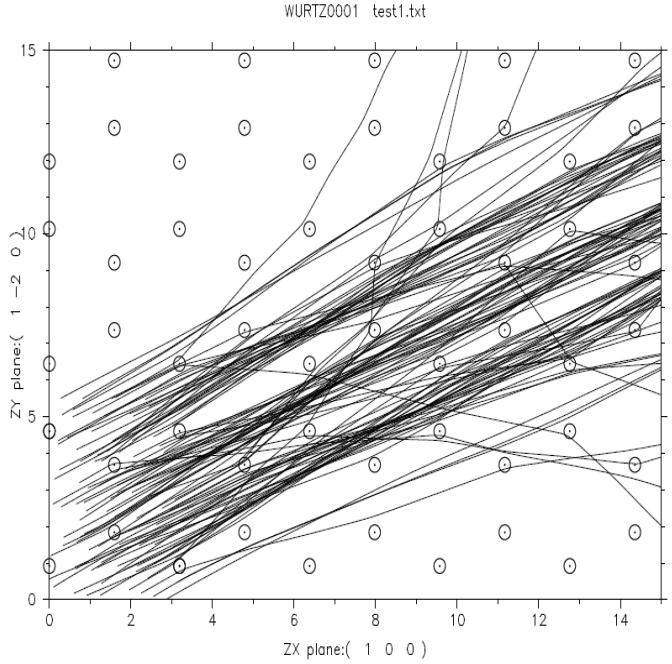
Ion tracks x-y (track.exe)

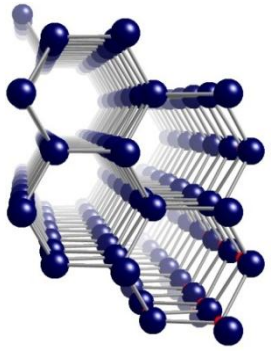
(0,0)



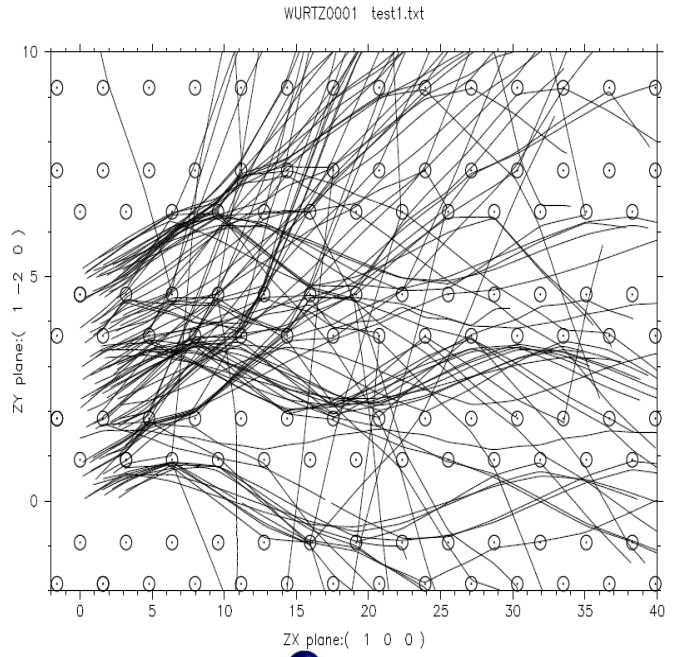


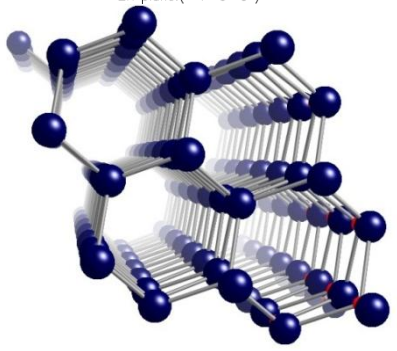
(1.5,30)





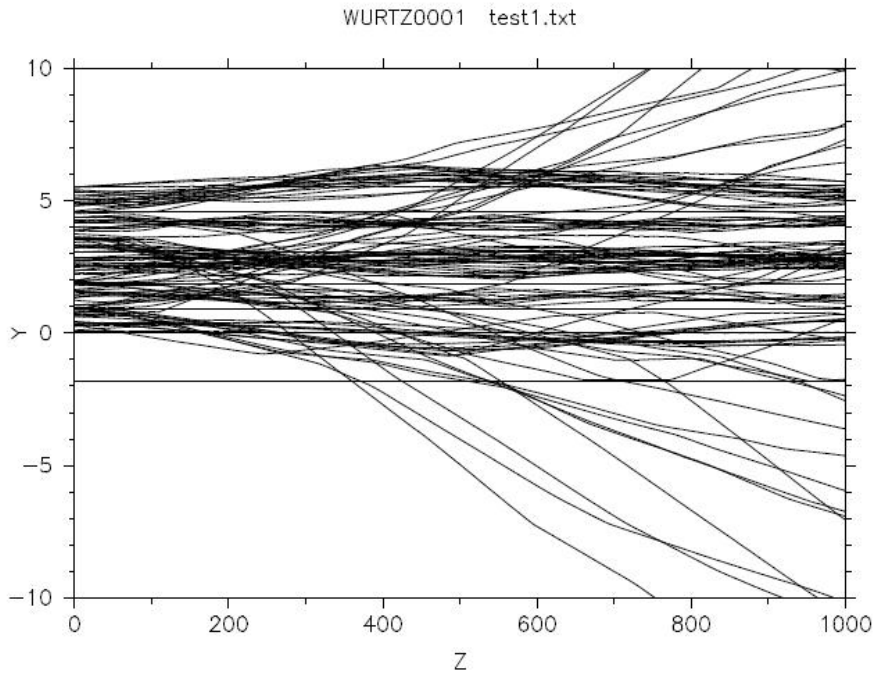
(1.5,10)

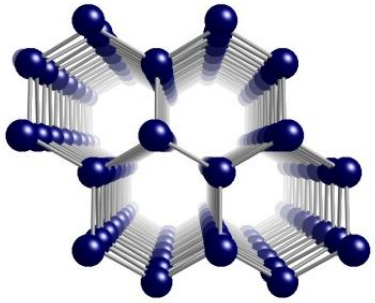




Ion tracks z-y (ztrack.exe)

(1.5,0)





Lattice Site Location: YIMP

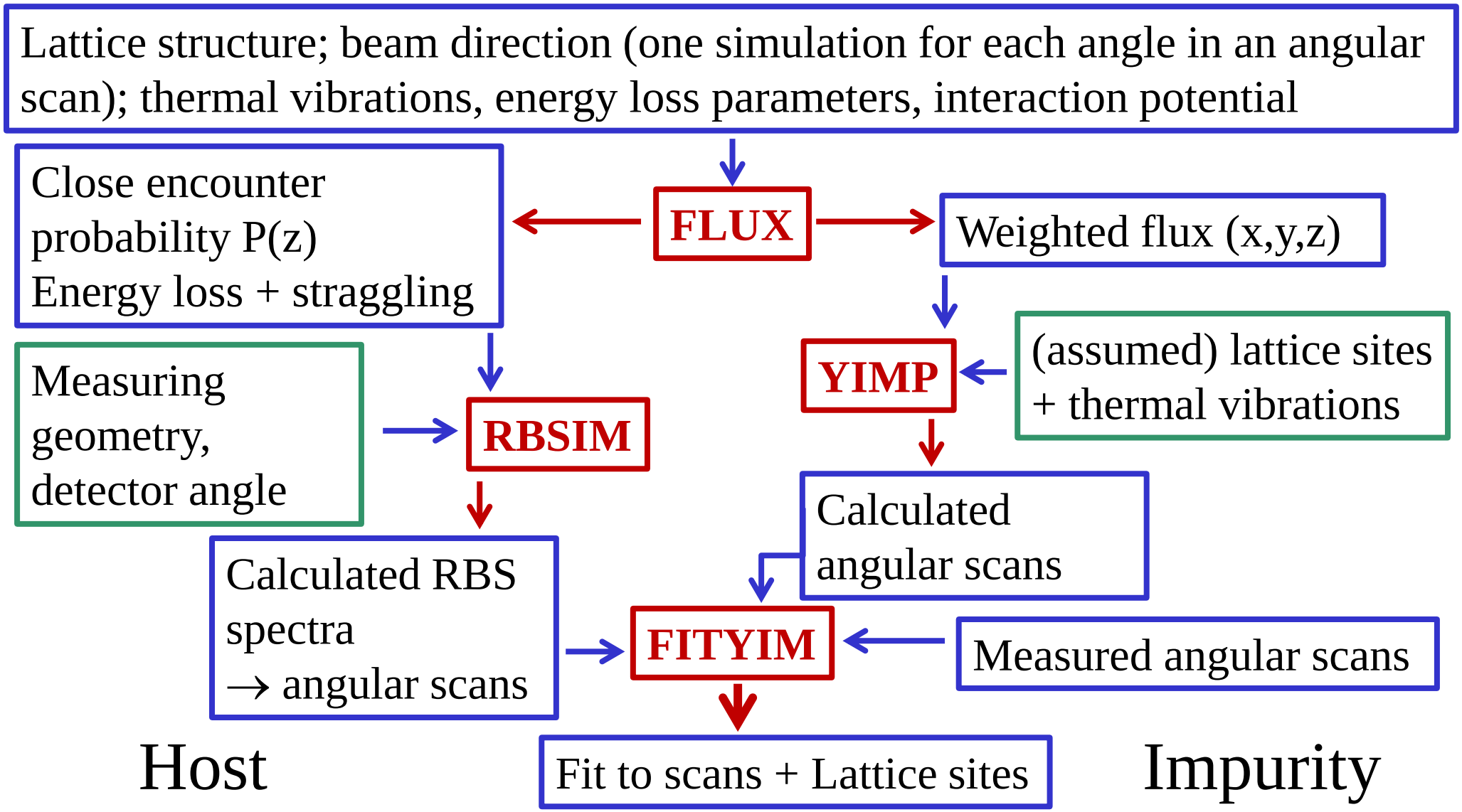
- YIMP uses as input the weighted flux distribution calculated by FLUX (convolution of the flux density ρ(x,y,z) with the impurity depth distribution w(z))

- Calculate the yield for the impurity atoms (convoluting the distribution of assumed lattice sites (taking into account their thermal vibrations) with the weighted flux)

- YIMP sets-up a library of angular scans for different impurity sites which can then be used in a fitting procedure.

- Advantage: Time-consuming FLUX MC calculation is only done once!

Lattice Site Location: YIMP



YIMP Input file for <0001> GaN

```
test2.flx
test2.ymp
WURTZ0001
152,-.075,
4,1,
1,
0,0.3333333,0,0,1,
1,0.6666666,0,0,1,
0,-0.3333333,0,0,1,
1,1.3333,0,0,1,
0
```

→ FLUX-file used as input
Name of the YIMP out-put file

→ Mass number of impurity (here Eu) and its vibration amplitude (Debye temperature can also be given)

→ x-y-coordinates of substitutional lattice sites and displacements dx and dy

YIMP Input file for <0001> GaN

```
152,-.1,
4,1,
1,
0,0.3333333,0,0,1,
1,0.6666666,0,0,1,
0,-0.3333333,0,0,1,
1,1.3333,0,0,1,
0
```

→ New lattice site with higher vibration amplitude

YIMP Input file for <0001> GaN

```
152,-.2,
4,1,
1,
0,0.3333333,0,0,1,
1,0.6666666,0,0,1,
0,-0.3333333,0,0,1,
1,1.3333,0,0,1,
0
```

→ New lattice site with yet a higher vibration amplitude

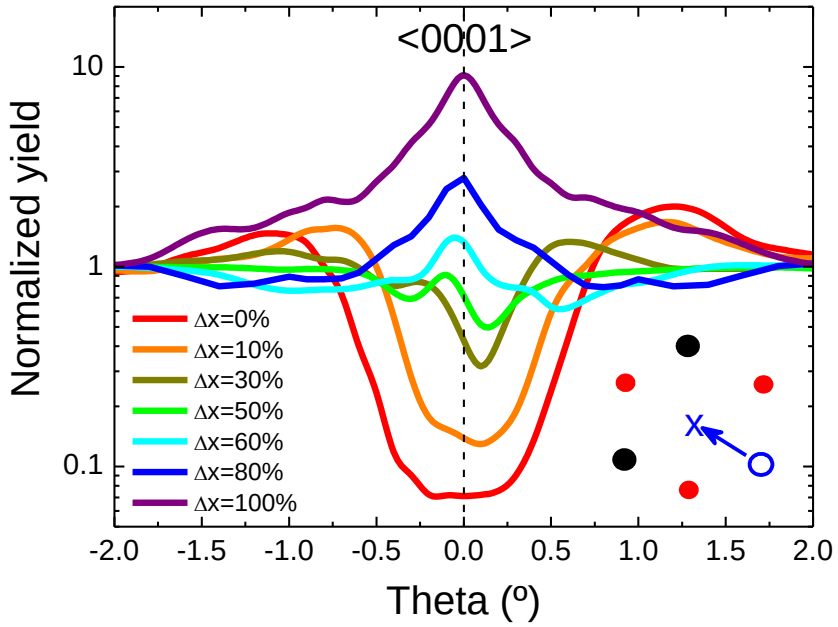
YIMP Input file for <0001> GaN

```
152,-.075,
4,1,
1,
0,0.3333333,0,0.7,1,
1,0.6666666,-1,0.3,1,
0,-0.3333333,0,0,1,
1,1.3333,0,0,1,
1
0,0,0,
```

→ New lattice site with displacements dx and dy shifting the impurity inside the channel

Lattice Site Location: YIMP

Impurity shifted from substitutional site towards the centre of the channel



→ Flux peaking when the impurity site coincides with areas of increased particle flux

FLUX Applications and Limits

Applications:

- Strain
- Epitaxy (mosaicity)
- Impurity lattice site location
- …many more (see literature list at the FLUX webpage) e.g. I did not talk much about planar channelling.

Limitations:

- FLUX assumes a perfect crystal (some possibility to include vacancies and one can play with the vibration amplitude)
- MC approach is only used for the incoming beam (outgoing beam is treated as random)
- FLUX looks for the scattering partner only within each plane and not in 3D