From McChasy 1 to McChasy 2

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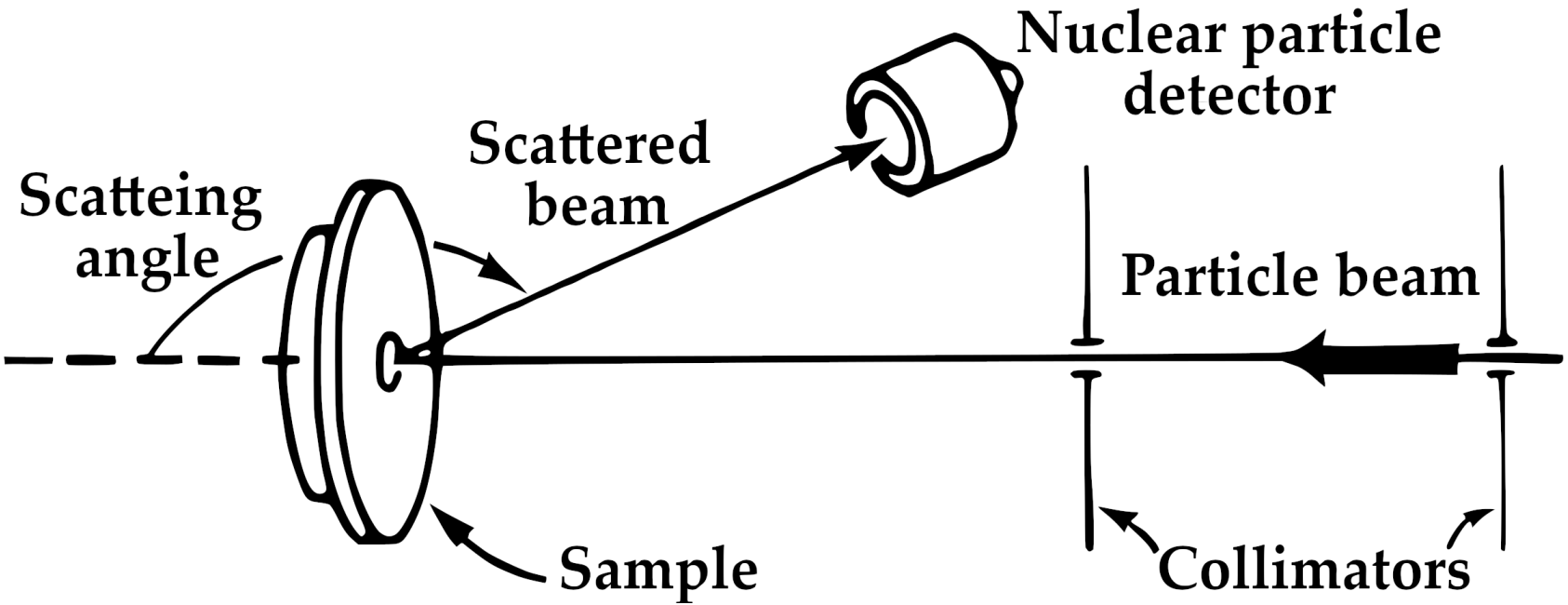
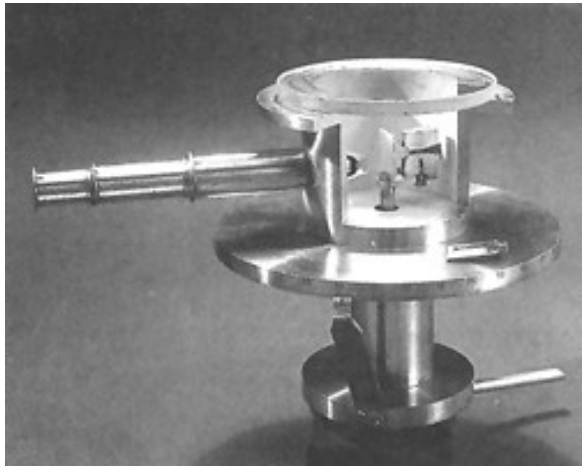
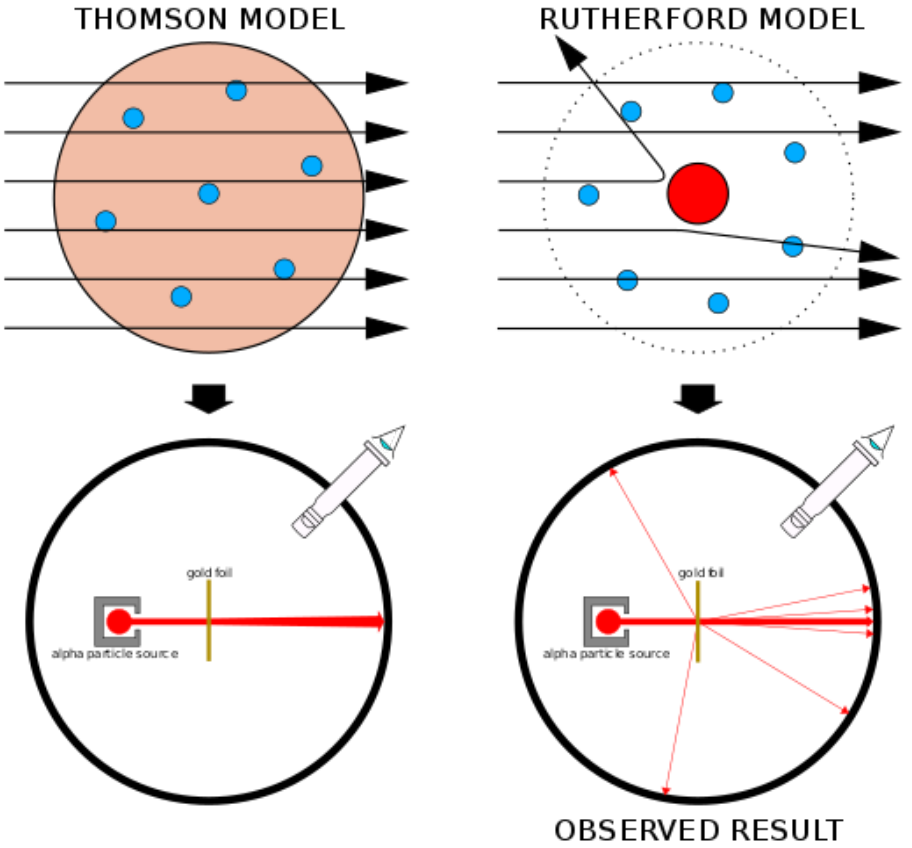
New reactor concepts and safety analyses for the Polish Nuclear Energy Program
POWR.03.02.00-00.I005/17

Rutherford backscattering spectrometry



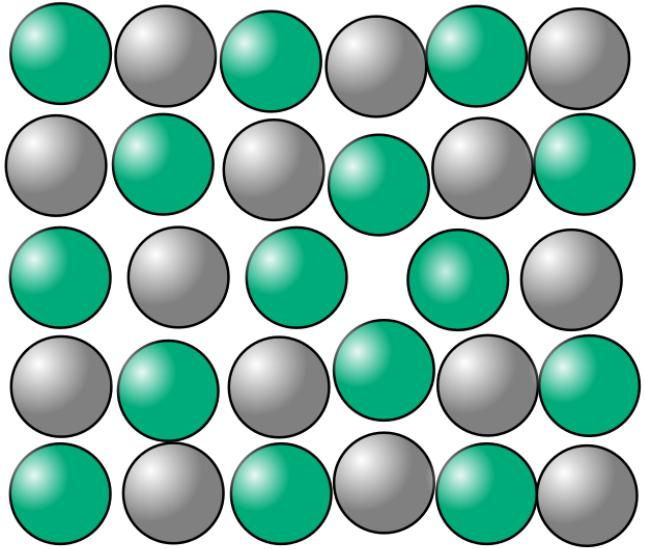
Geiger–Marsden experiment





Why RBS?

Information about the depth concentration of the scattering centers.



What kind of RBS?

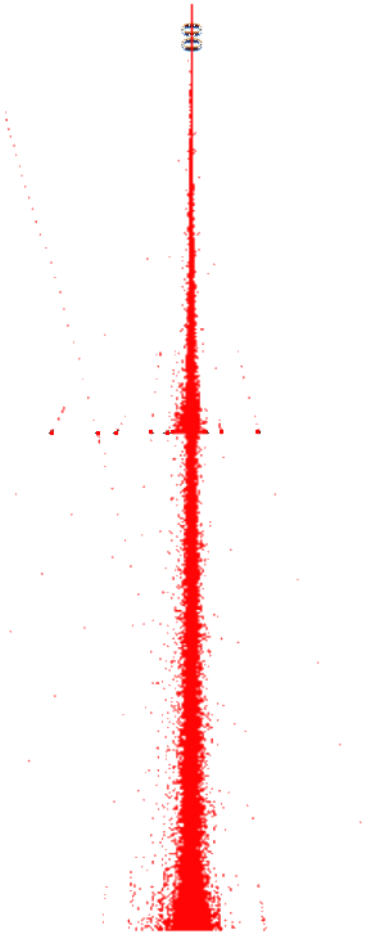
RBS/C - Rutherford backscattering/channeling

Ion beam channeling - incoming ions are guided into the channel or plane. Side efect: decrease of the backscattered yield.

Main crystallographic axes (001, 011, 111)

RBS/C

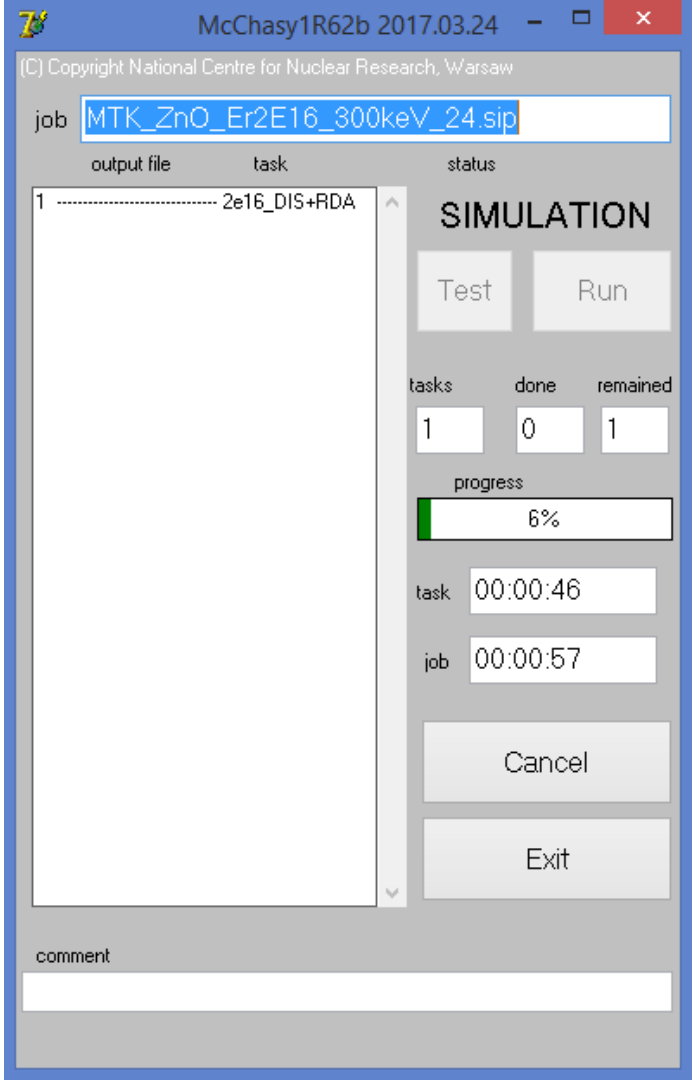
From channeling measurements, information is obtained concerning the crystalline quality of the lattice (i.e. defects), the elastic strain and the azimuthal orientation.



Doktor Lech Olgierd Nowicki

Graphical interface for McChasy.

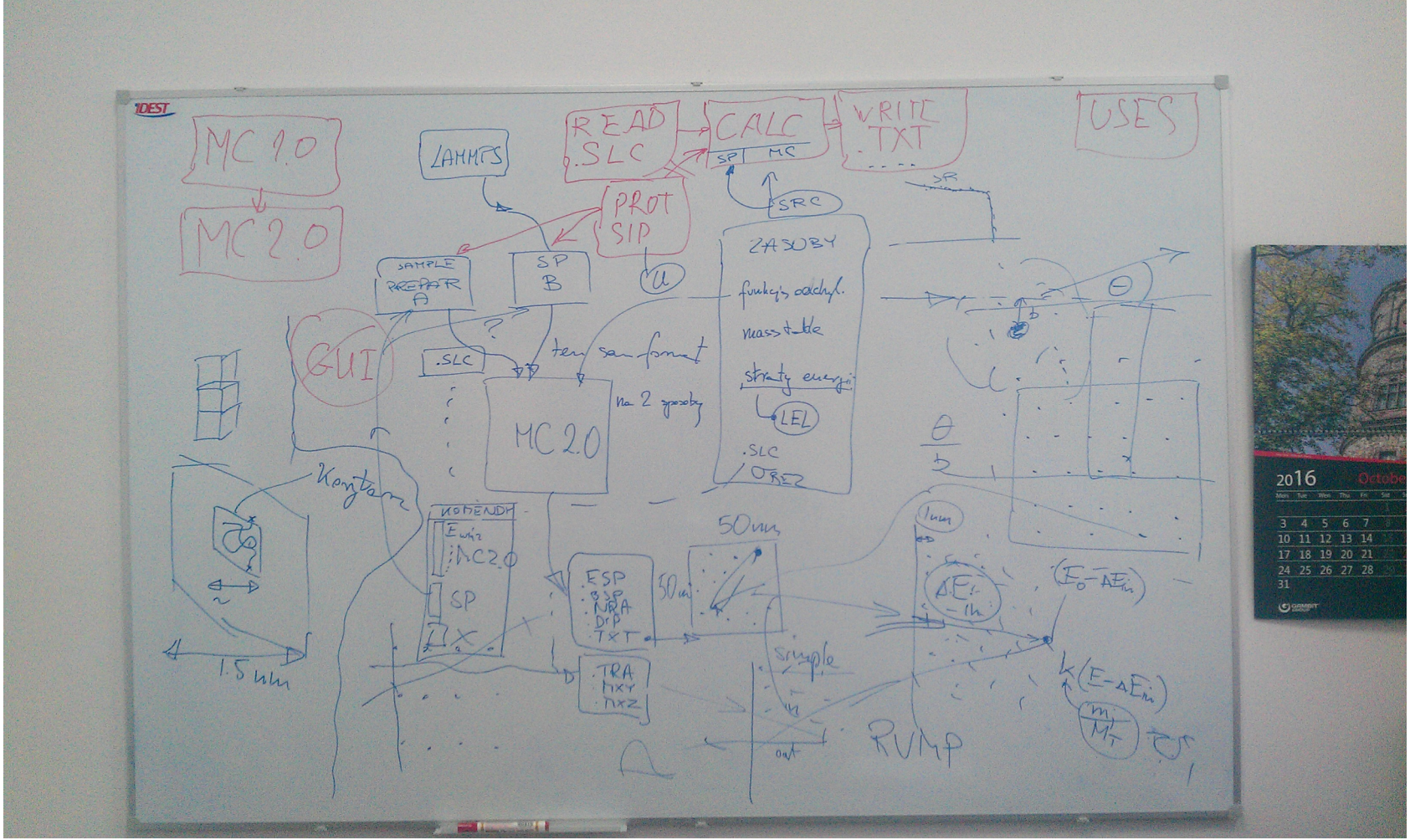
Created in Delphi
First version of McChasy 1996?
McChasy
Monte Carlo
CHanneling SYmulation



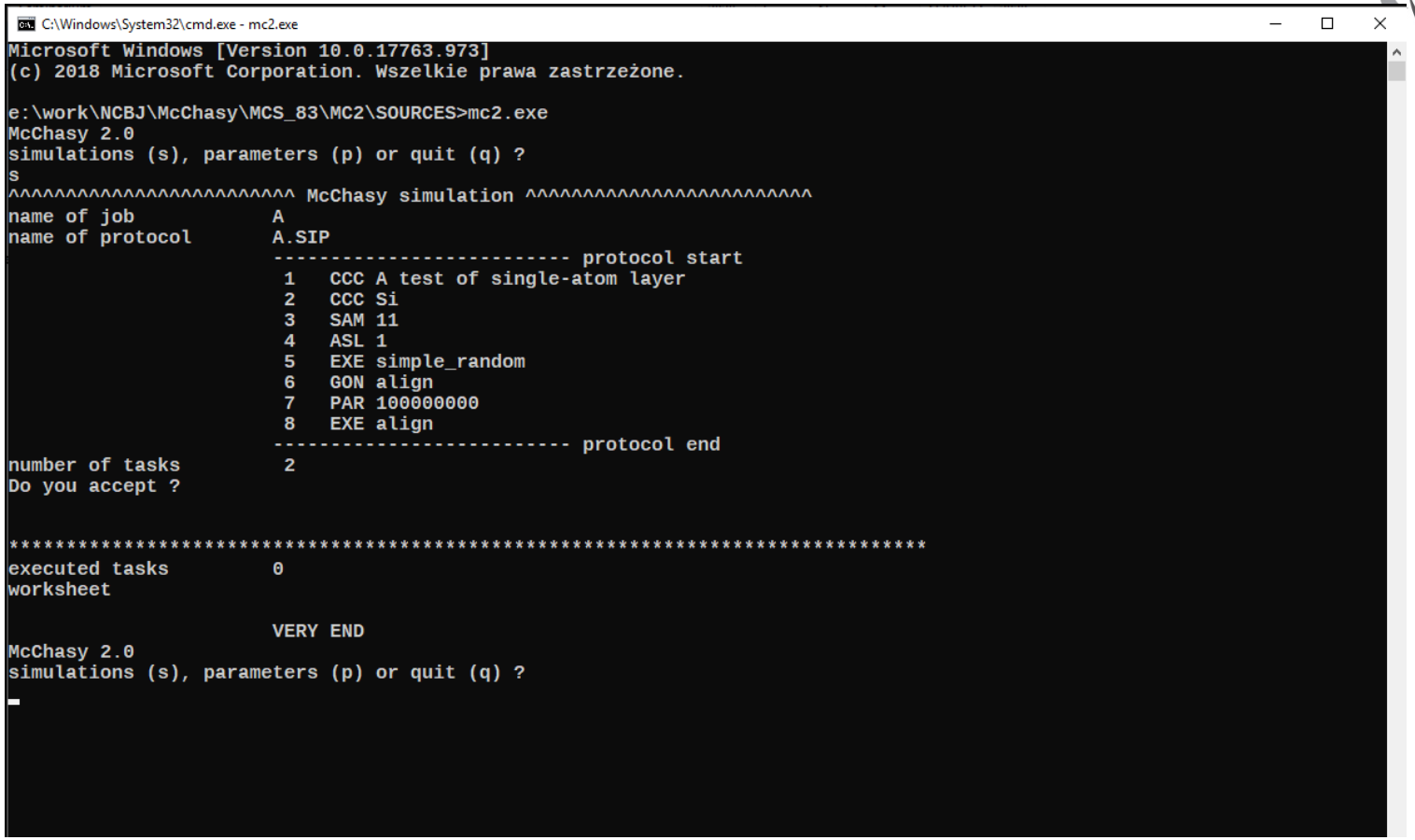
Simulation protocol

pC.SPP A3.SIP

```
CCC A1
CCC test probek
CCC
PAR 64
*** **********************
SAM 112
GON off
EXE 112R
GON align
EXE 112A
*** **********************
SAM 113
GON off
EXE 113R
GON align
EXE 113A
*** **********************
SAM 113
GON off
EXE 113R
GON align
EXE 113A
```


MC 1.0
MC 2.0
LAMMPS
READ .SLC
CALC
SP
MC
WRITE .TXT
USES
PROT SIP
SRC
ZASOBY
funkcje oddział.
mass table
straty energii
LEL
.SLC
ORER
SAMPLE PREPAR A
SP B
GUI
.SLC
ten sam format
na 2 sposoby
MC 2.0
Kontakt
KONIEC
Ewiz
MC2.0
SP
ESP
.SSP
.NRA
.DAT
.TXT
.TRA
.TXY
.TXZ
50 nm
50 nm
1 nm
1.5 nm
simple
RUMP
SR

McChasy 2


C:\Windows\System32\cmd.exe - mc2.exe
Microsoft Windows [Version 10.0.17763.973]
(c) 2018 Microsoft Corporation. Wszelkie prawa zastrzeżone.
e:\work\NCBJ\McChasy\MCS_83\MC2\SOURCES>mc2.exe
McChasy 2.0
simulations (s), parameters (p) or quit (q) ?
s
^^^^^^^^^^^^^^^^^^^^^^^^^ McChasy simulation ^^^^^^^^^^^^^^^^^^^^^^^^^
name of job A
name of protocol A.SIP
---------- protocol start
1 CCC A test of single-atom layer
2 CCC Si
3 SAM 11
4 ASL 1
5 EXE simple_random
6 GON align
7 PAR 100000000
8 EXE align
---------- protocol end
number of tasks 2
Do you accept ?
****
executed tasks 0
worksheet
VERY END
McChasy 2.0
simulations (s), parameters (p) or quit (q) ?

free pascal

OPEN SOURCE COMPILER FOR PASCAL AND OBJECT PASCAL

INTRODUCTION

Overview

Free Pascal is a 32, 64 and 16 bit professional Pascal compiler. It can target many processor architectures: Intel x86 (including 8086), AMD64/x86-64, PowerPC, PowerPC64, SPARC, ARM, AArch64, MIPS and the JVM. Supported operating systems include Linux, FreeBSD, Haiku, Mac OS X/iOS/iPhoneSimulator/Darwin, DOS (16 and 32 bit), Win32, Win64, WinCE, OS/2, MorphOS, Nintendo GBA, Nintendo DS, Nintendo Wii, Android, AIX and AROS. Additionally, support for the Motorola 68k architecture is available in the development versions.

Latest News

July 20, 2019

FPC has gained several new features lately:

- Multiple helper types can now be active at the same time
- Support has been added for custom attributes
- The compiler can now generate LLVM bitcode for select platforms (Darwin/x86-64, Linux/x86-64, Linux/AArch64, Linux/ARMHF)

The next FPC release, version 3.2, is planned for later this year. While it will not have support for the above list, it will have its own collection of new features and fixes!

June 8, 2018

Today FPC celebrates its 25th birthday ! 25 years have passed since 8 june 1993, and FPC still does not only exists, but is more alive and kicking than ever!

May 28, 2018

As required by the European GDPR, we have published a privacy statement

November 28th, 2017

FPC version 3.0.4 has been released!

This version is a point update to 3.0 and contains bugfixes and updates packages, some of which are high priority.

There is a list of changes that may break backward compatibility. You can also have a look at the FPC 3.0.4 documentation.

Downloads are available at the download section.

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Authors
Credits
Links/mirrors
TOOLS
Tools
Delp
FPCMake
H2Pas
PPDep
PPUDump

Sample protocol

pC.SPP A3.SIP

```
*** *************** U02 ****************
TGT U02
*** ************************************
KLM 001
*** ************************************
SIZ brick 30 10
CCC U02-001 brick
SAM 120
SIZ cone 10 50 10
CCC U02-001 cone
SAM 121
*** ************************************
KLM 011
*** ************************************
SIZ brick 30 10
CCC U02-011 brick
SAM 122
SIZ cone 10 50 10
CCC U02-011 cone
SAM 123
*** ************************************
KLM 111
*** ************************************
SIZ brick 30 10
CCC U02-111 brick
SAM 124
SIZ cone 10 50 10
CCC U02-111 cone
SAM 125

```

Random – amorphous sample

Virgin – non implanted

Alingment (001)

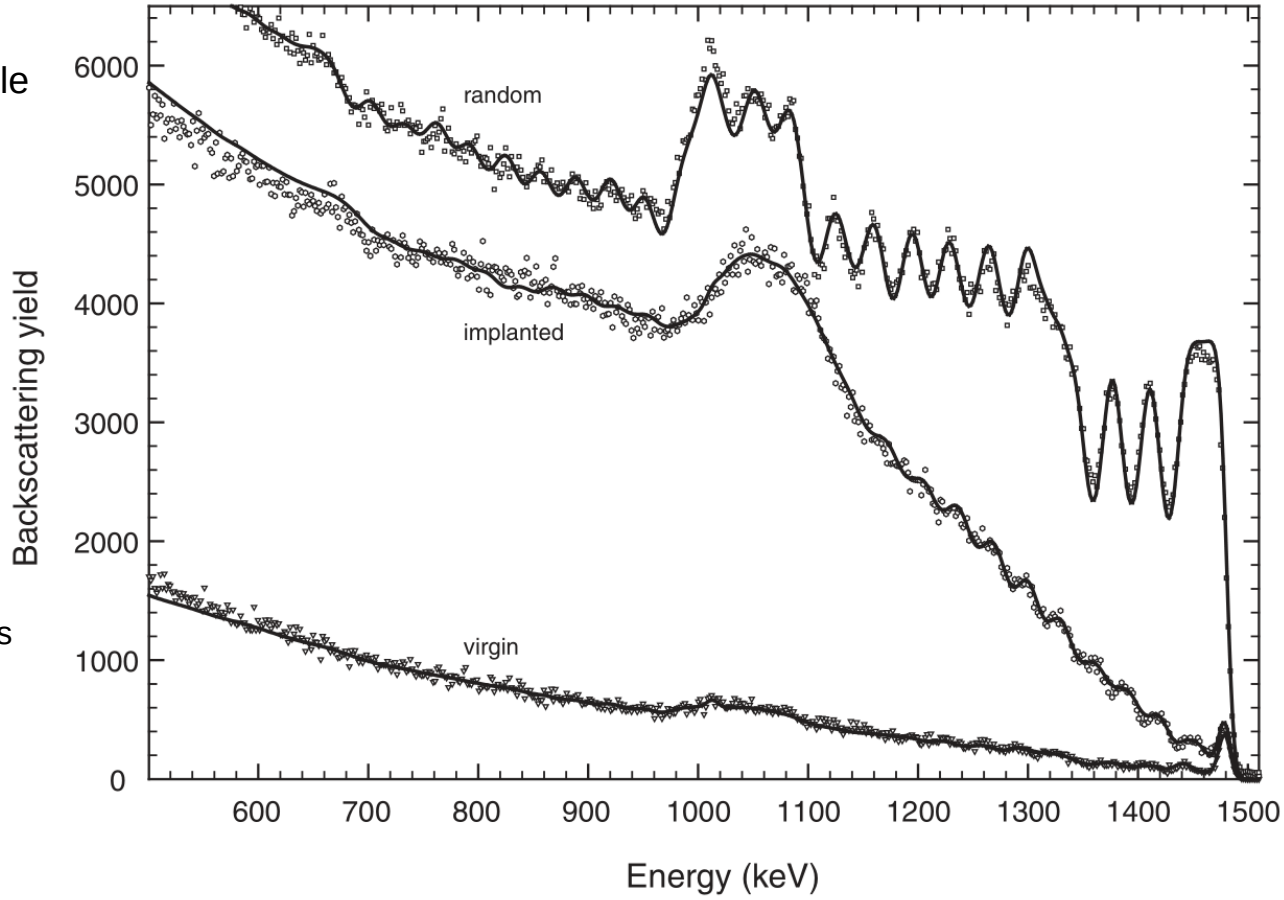
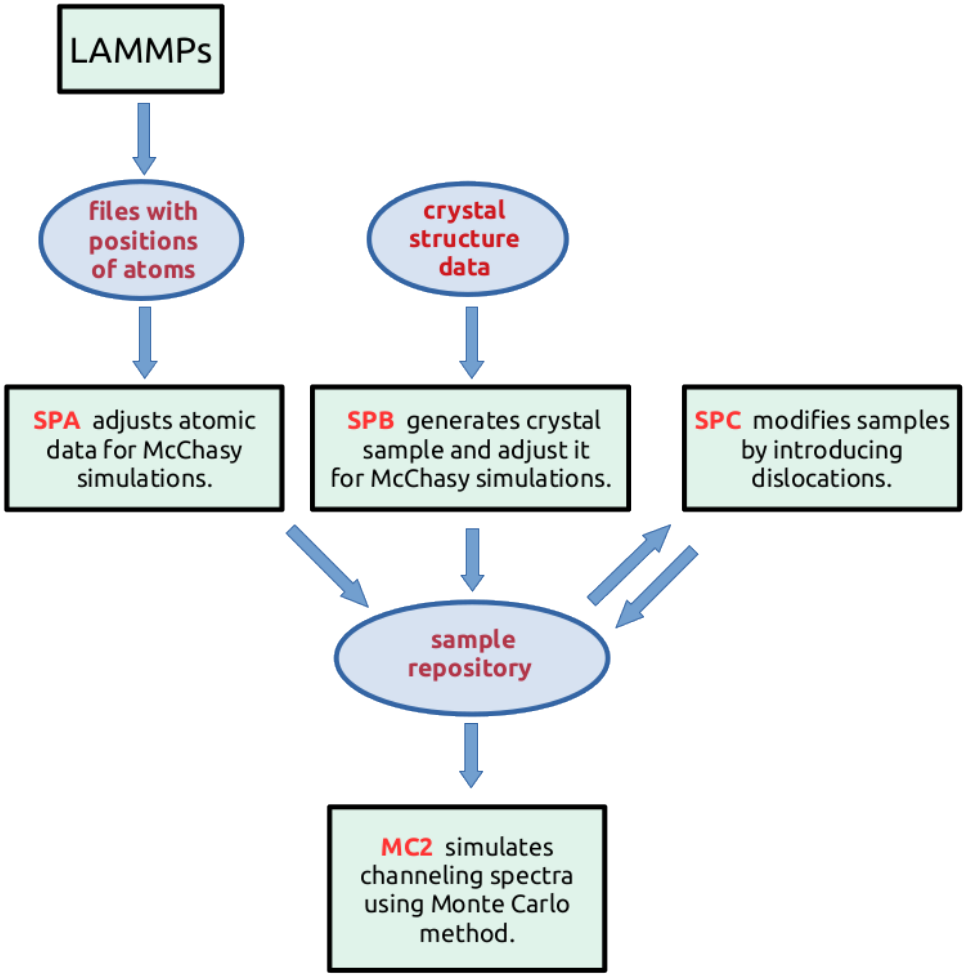


Fig. 2. He backscattering spectra of InGaAsP/InP superlattice.

L. Nowicki, A. Turos, R. Ratajczak, A. Stonert, F. Garrido. Modern analysis of ion channeling data by Monte Carlo simulations. Nuclear Instruments and Methods in Physics Research B 240 (2005) 277–282.

McChasy 2

Present status

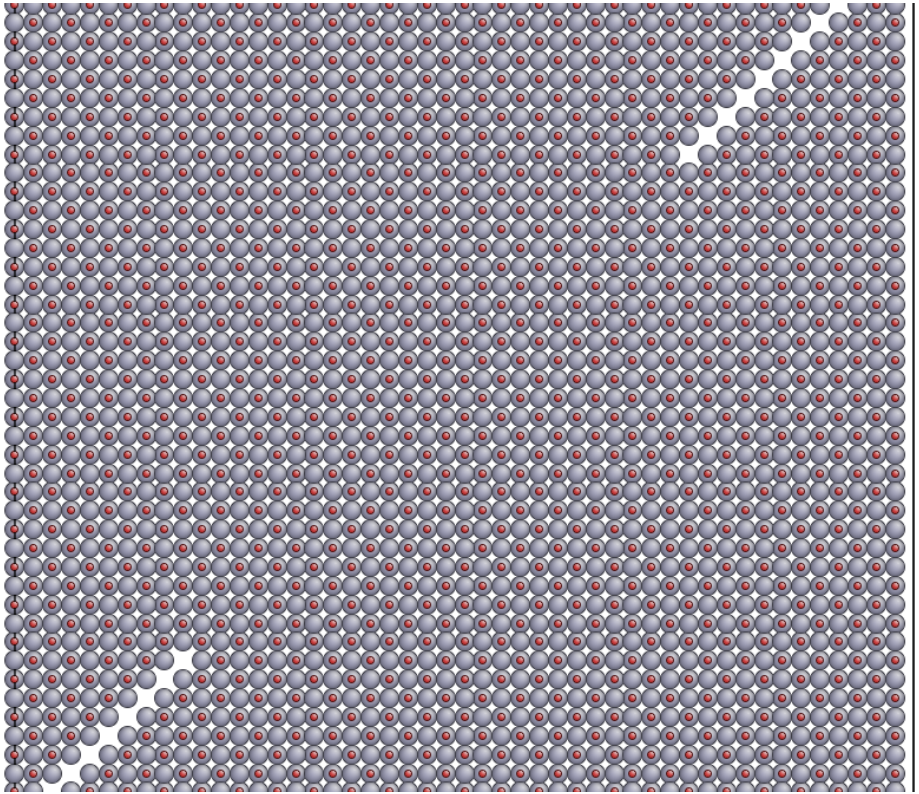


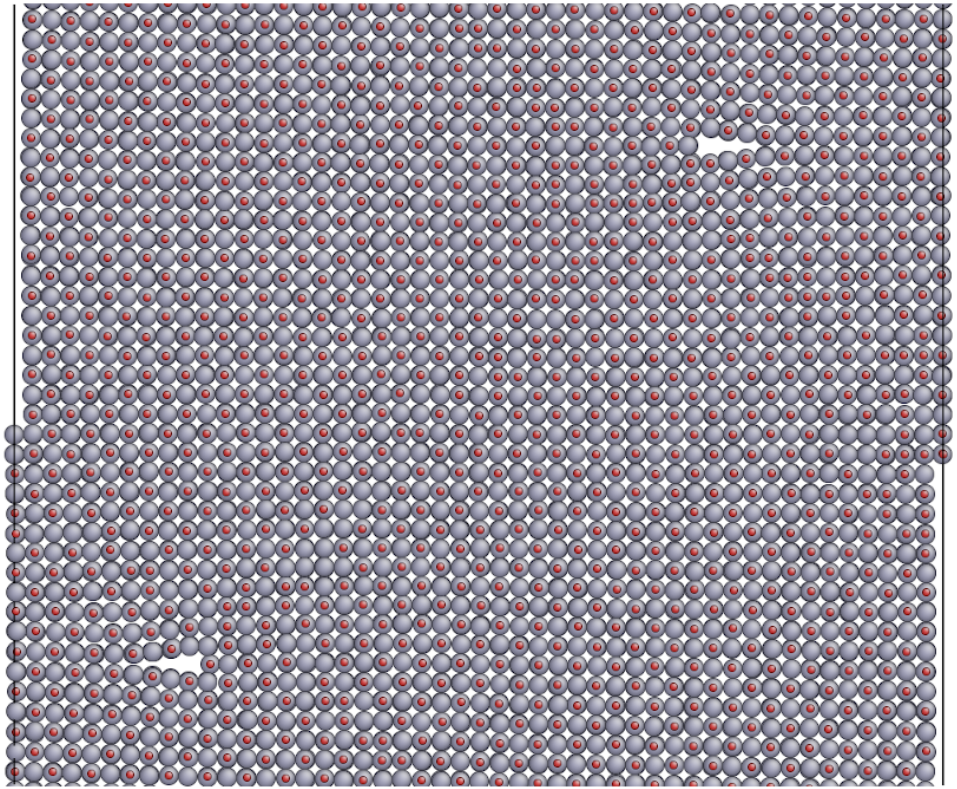
Termodynamiczne właściwości ceramiki z defektami struktury w obecności promieniowania

Alain Chartier, Orest Dorosh, Jacek Jagielski

16.04.2014 Świerk

Dislocation with molecular dynamics





Compilation

Optimisation

```
$ fpc -O4 mc2.pas
```

McChasy2: new Monte Carlo RBS/C simulation code designed for use with large crystalline structures.

Lech Nowicki[1)], Jacek Jagielski[1,2,*)], Cyprian Mieszczyński[1)], Kazimierz Skrobas[1,4)], Przemysław Jóźwik[1,3)], Orest Dorosh[1)]

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2) Institute for Electronic Materials Technology, Wolczynska 133, 01-926 Warszawa, Poland
3) IPFN, Instituto Superior Técnico, Universidade de Lisboa, Estrada Nacional 10, Bobadela, 2695-066, Portugal
4) Institute of High Pressure Physics PAS, ul. Sokolowska 29/37, 01-142 Warsaw Poland

**) Corresponding author*

Summary

	McChasy	McChasy 2
Language	Delphi	Freepascal, C++
Sample	SPB	SPB, LAMMPS
Number of atoms	<1000	>100000
Defects	Difficult	Not so difficult

Thank you for attention

NATIONAL CENTRE FOR NUCLEAR RESEARCH
ŚWIERK

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