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IBA Intro III Introduction to codes

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IBA Intro III

Introduction to codes

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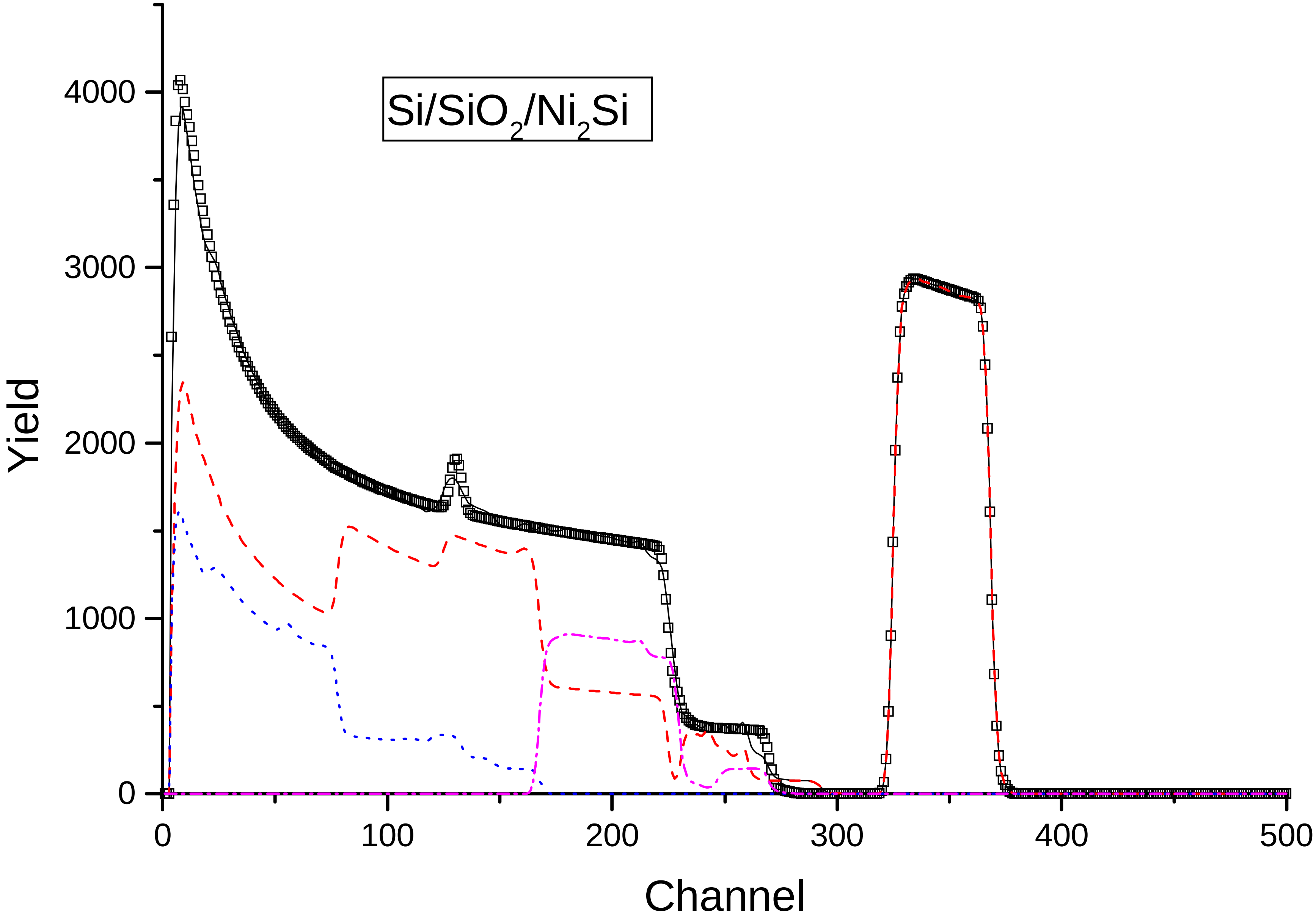
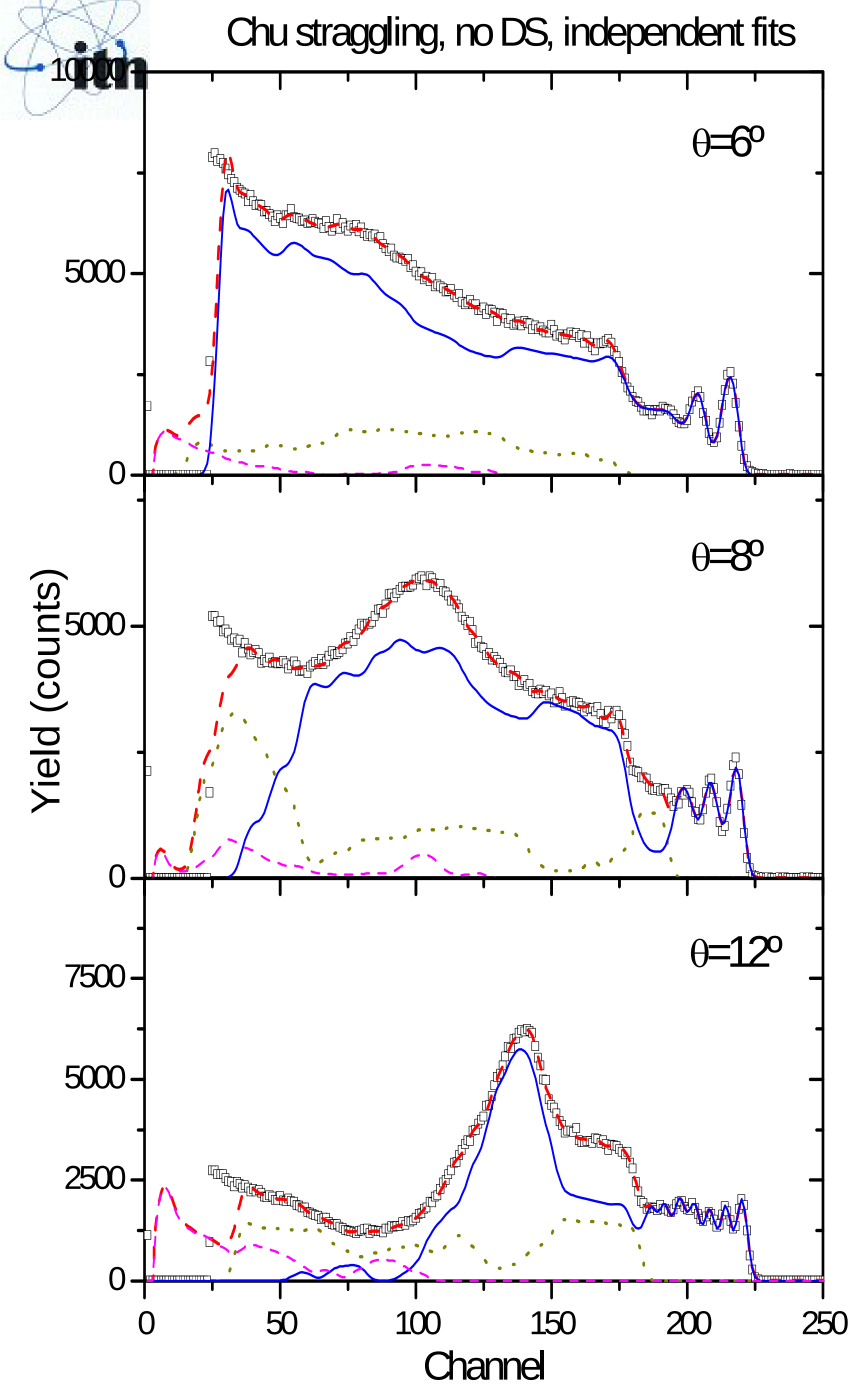
Overview

- Introduction
- The IAEA review and intercomparison of IBA software, Handbook of Modern Ion Beam Analysis (2nd edition)
- Types of codes
- Design and capabilities of selected codes
- Accuracy of codes and experiments



Si/SiO2/Ni2Si
Yield
4000
3000
2000
1000
0
0
100
200
300
400
500
Channel



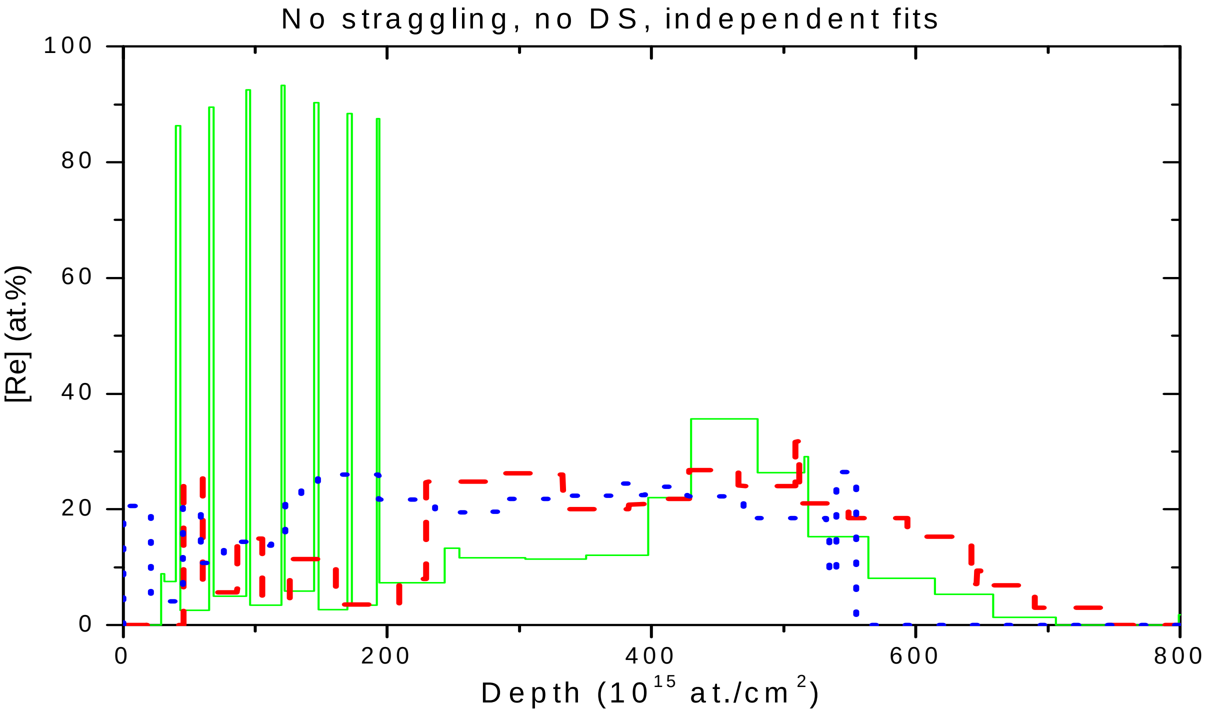
Sample:

Si/Re 50 Å/(Co 20Å/Re 5Å)$_{16}$

1 MeV He^{+} beam, 160º Cornell

Fit the spectra one by one:

Perfect fits with no meaning



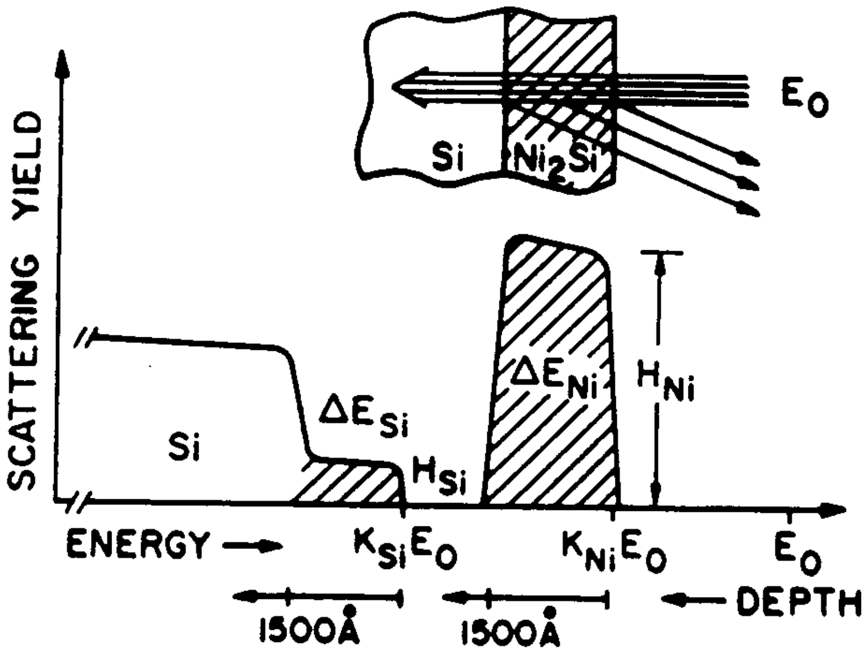
Data analysis $\neq$ software

- Ambiguous data (different sample structures lead to same fit)
- Limited knowledge of experimental conditions (charge, solid angle, angle of incidence and detection, beam energy, FWHM,…)
- Limited knowledge of basic data (stopping, cross section)
- Surprises in sample (roughness, unexpected elements, roughness, …)
- Limited knowledge of relevant physics

$\Rightarrow$ Good fits can be meaningless

"It cannot be overemphasized that software is an aide to data analysis, and does not replace the judgment of the analyst. Software that is not correctly used, or used outside its scope of application, leads to wrong data analysis."

Manual analysis



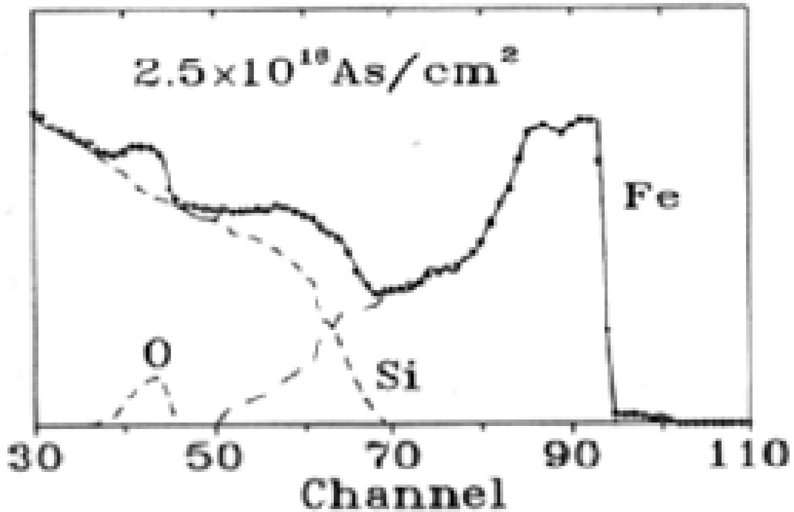
$$\frac{N_{Ni}}{N_{Si}} = \frac{A_{Ni}}{A_{Si}}\frac{\sigma_{Si}}{\sigma_{Ni}} = \frac{H_{Ni}}{H_{Si}}\frac{\Delta E_{Ni}}{\Delta E_{Si}}\left(\frac{Z_{Si}}{Z_{Ni}}\right)^2$$

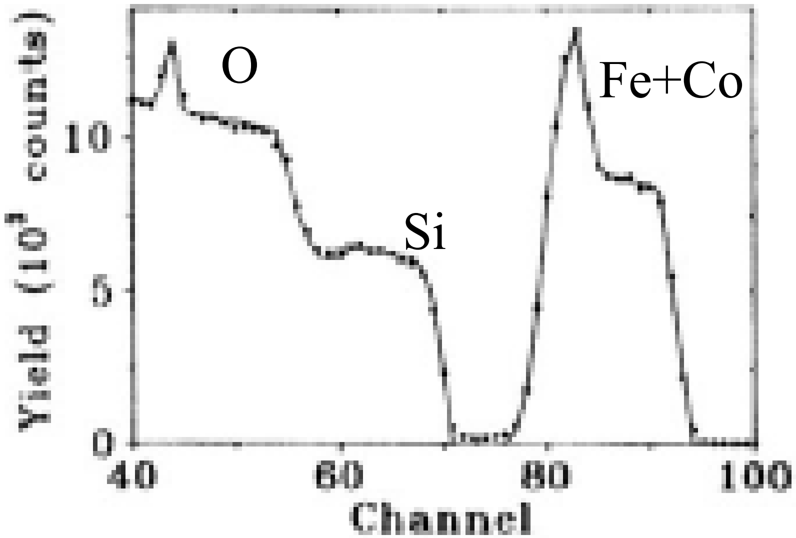
H_{Ni}=2.3 cm, ΔE_{Ni}=1.1 cm

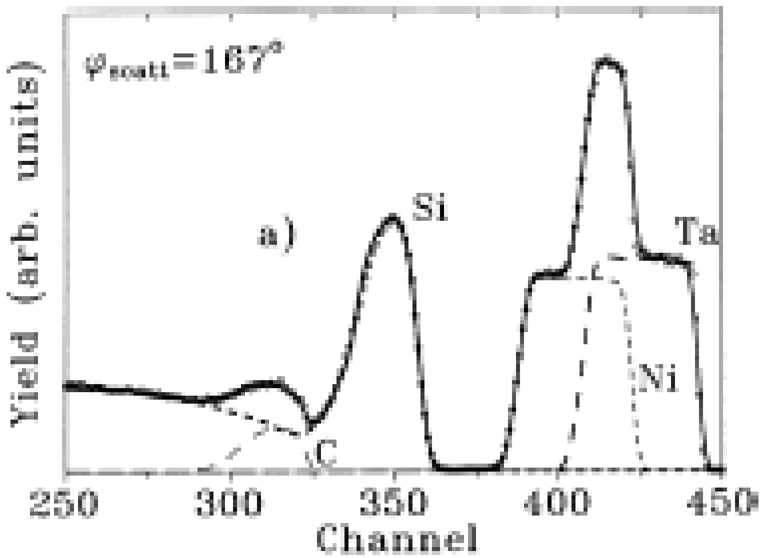
H_{Si}=0.35(5) cm, ΔE_{Si}=0.9 cm

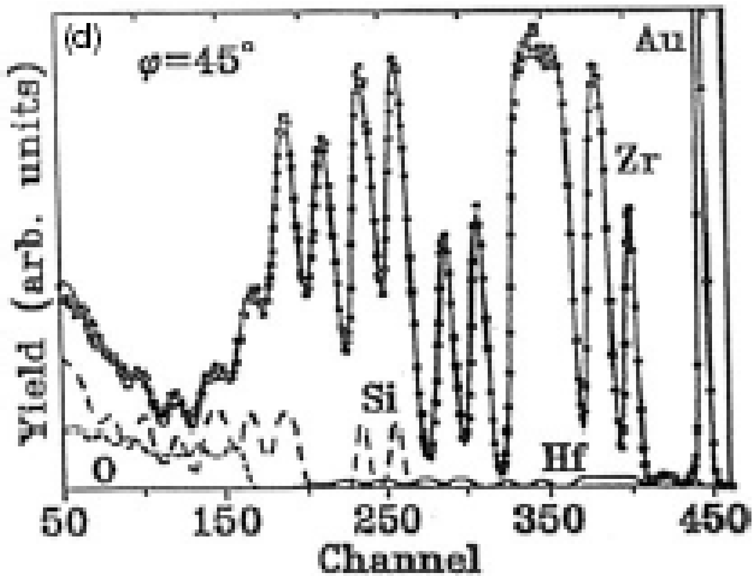
$\therefore N_{Ni}/N_{Si} = 2.0(3) \Rightarrow Ni_2Si$

Why use software?


2.5×10¹⁶As/cm²
Fe
O
Si
30
50
70
90
110
Channel


O
Fe+Co
Si
Yield (10³ counts)
10
5
0
40
60
80
100
Channel


φscatt=167°
Yield (arb. units)
a)
Si
Ta
Ni
C
250
300
350
400
450
Channel


(d)
φ=45°
Au
Zr
Yield (arb. units)
Si
O
Hf
50
150
250
350
450
Channel

Why use software?

- Huge efficiency gains in the analysis process
- Enables data analysis by non-experts (including students and casual users)
- Design experiments
- Education (scrutinise characteristics of various ion beam techniques)
- Help recognise limitations of data and of knowledge

- Implementation of advanced physics and models widens the range of samples that can be studied and information that can be derived

The IAEA review of IBA software

Status of IBA data analysis and simulation software

E. Rauhala, N. P. Barradas, S. Fazinic, M. Mayer, E. Szilágyi, M. Thompson
Nucl. Instrum. Methods Phys. Res. B244 (2006) 436-456.

- Contains no science
- Discusses the major issues concerning IBA data analysis and software
- Describes the status of 12 software packages
- Mentions some outstanding problems (some already solved)
- Has a list of 200+ references - a treasure for the IBA analyst!!!

The IAEA intercomparison exercise of IBA software

International Atomic Energy Agency intercomparison of Ion Beam Analysis software

N.P. Barradas, K. Arstila, G. Battistig, M. Bianconi, N. Dytlewski, C. Jeynes, E. Kótai, G. Lulli, M. Mayer, E. Rauhala, E. Szilágyi, M. Thompson Nucl. Instrum. Methods Phys. Res. B262 (2007) 281-303.

- 7 participating packages, including one MC code
- 28 simulations including RBS, EBS, ERDA, non resonant NRA, channelling, H, He and heavy ions
- 4 data sets from real samples

Handbook of Modern IBA 2nd edition

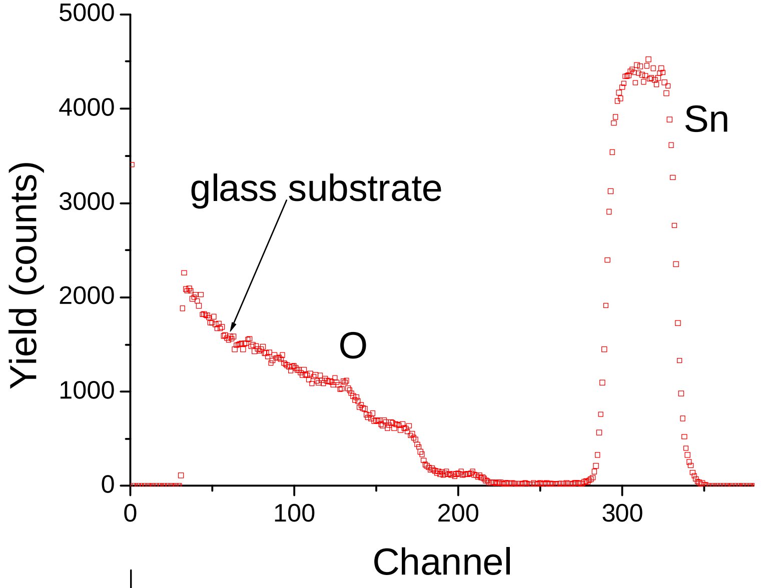
Chapter **Data analysis software for ion beam analysis**

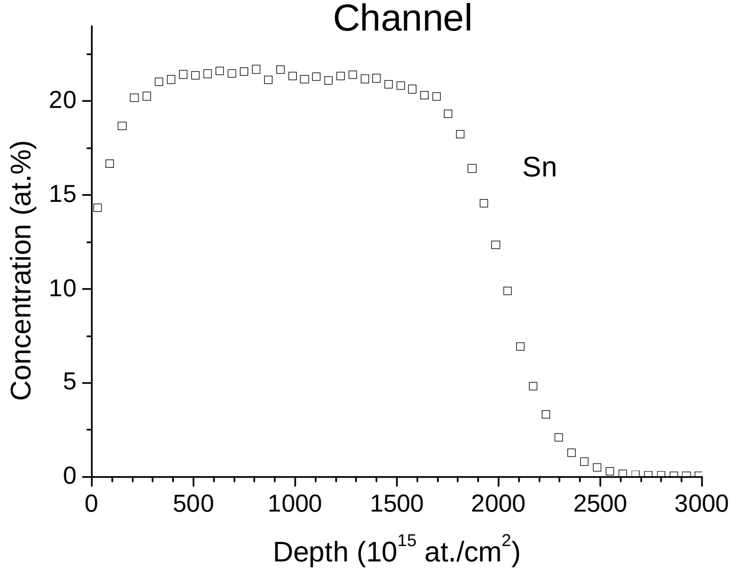
Nuno Pessoa Barradas and Eero Rauhala

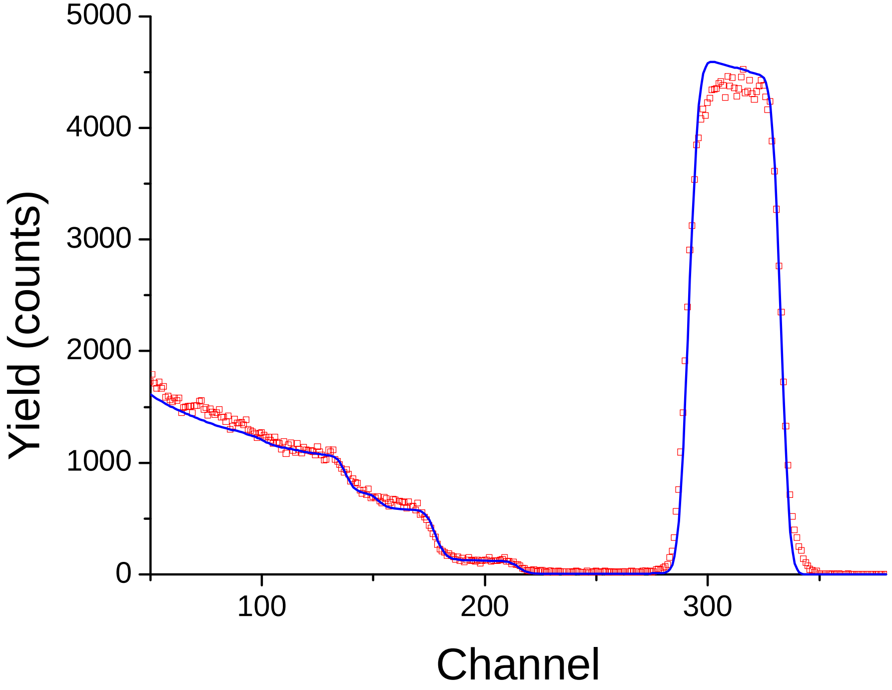
DEPTH	http://www.kfki.hu/~ionhp/doc/prog/wdepth.htm
FLUX	http://members.home.nl/p.j.m.smulders/FLUX/HTML/
GeoPIXE	http://www.nmp.csiro.au/GeoPIXE.html
GUPIX	http://pixe.physics.uoguelph.ca/gupix/main/
IBANDL	http://www-nds.iaea.org/ibandl/
Ion Beam Information System (includes links to several codes)	
	http://www.kfki.hu/~ionhp/
LibCPIXE	http://sourceforge.net/projects/cpixe
MSTAR	http://www.exphys.uni-linz.ac.at/stopping/
NDF	http://www.itn.pt/facilities/lfi/ndf/uk_lfi_ndf.htm
DataFurnace	http://www.ee.surrey.ac.uk/SCRIBA/ndf/
QXAS	http://www.iaea.org/OurWork/ST/NA/NAAL/pci/ins/xrf/pciXRFdown.php
RUMP	http://www.genplot.com
SigmaCalc	http://www-nds.iaea.org/sigmacalc/
SIMNRA	http://www.rzg.mpg.de/~mam/
SRIM	http://www.srim.org

Types of codes

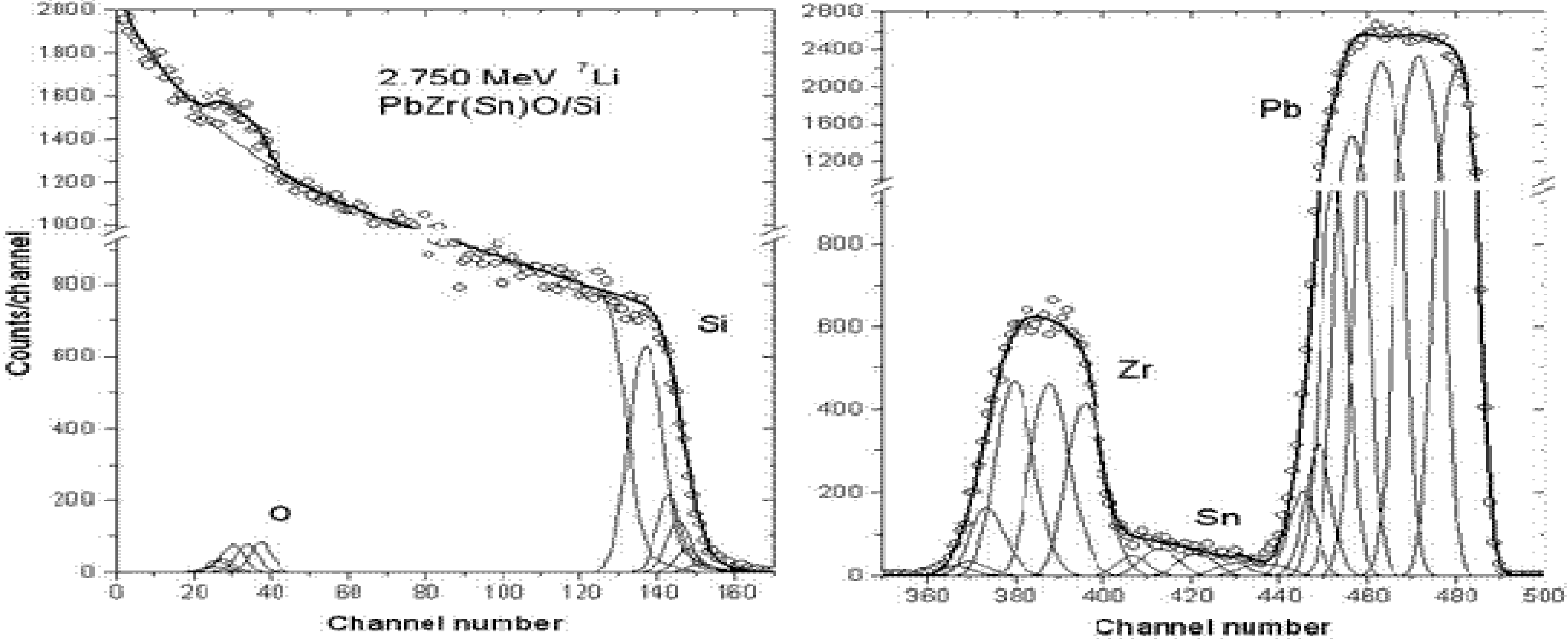
- Direct calculation vs. simulation

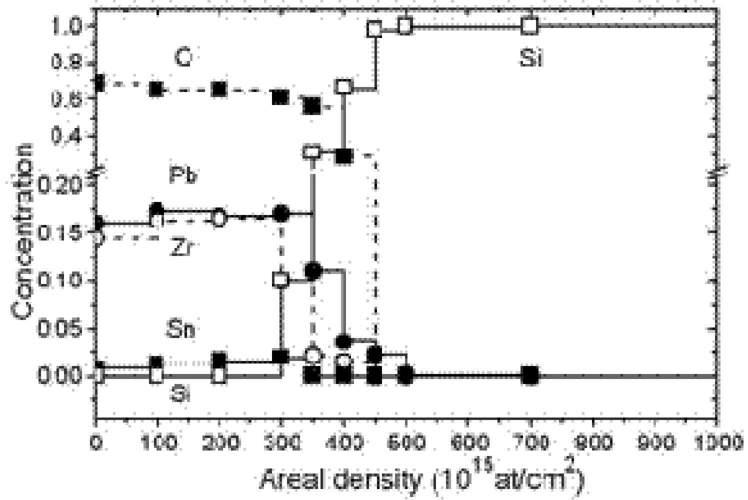






➢ Simulating composition changes by division into sublayers



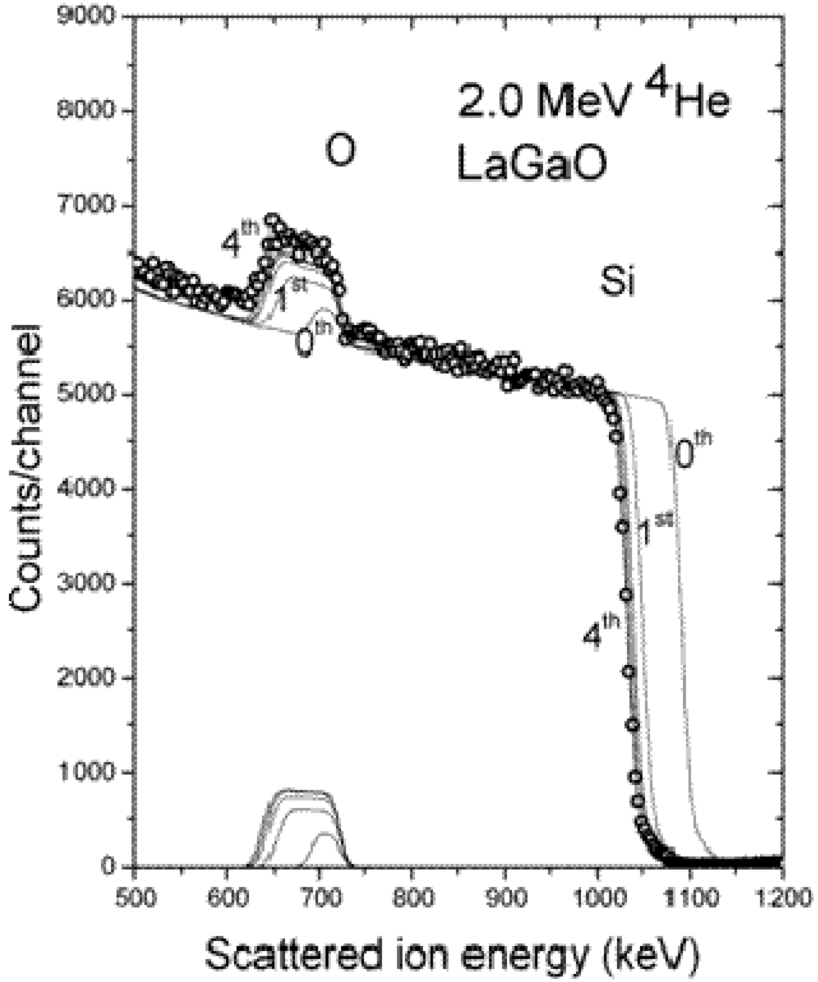


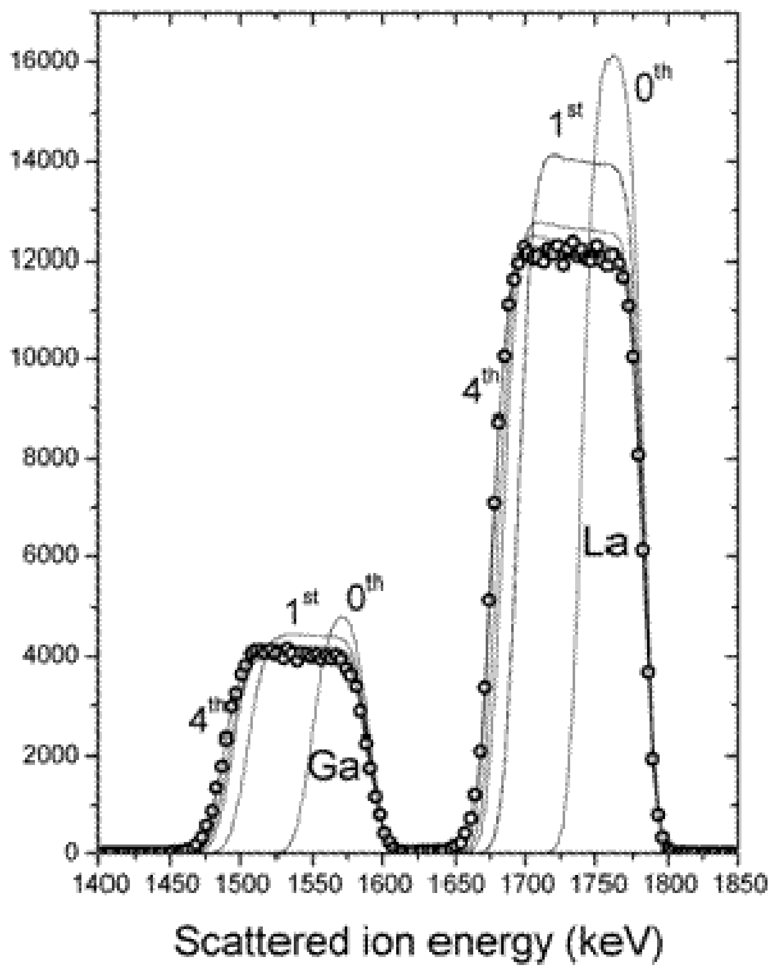
➢ (not so common) alternative: define continuous depth profiles

Types of codes

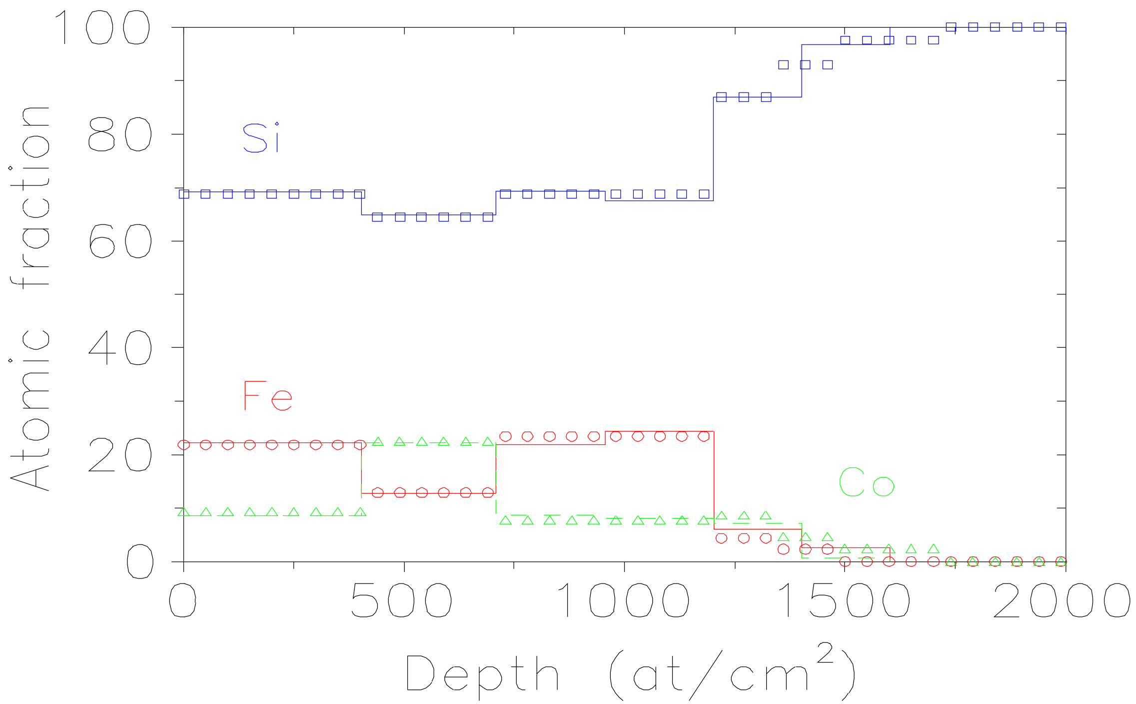
➢ Interactive vs. automated

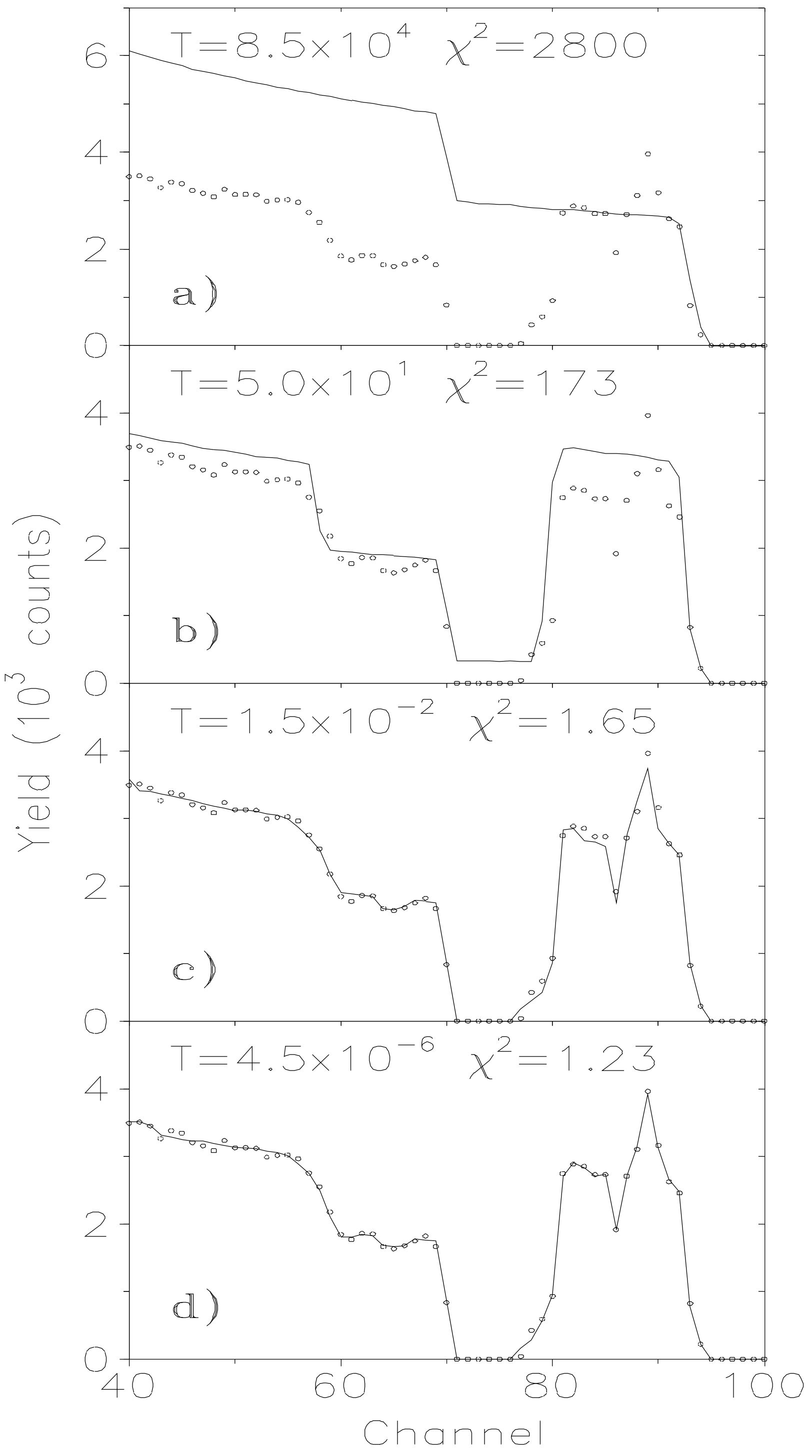
➢ Interactive





➢ Automated - Simulated annealing





Types of codes

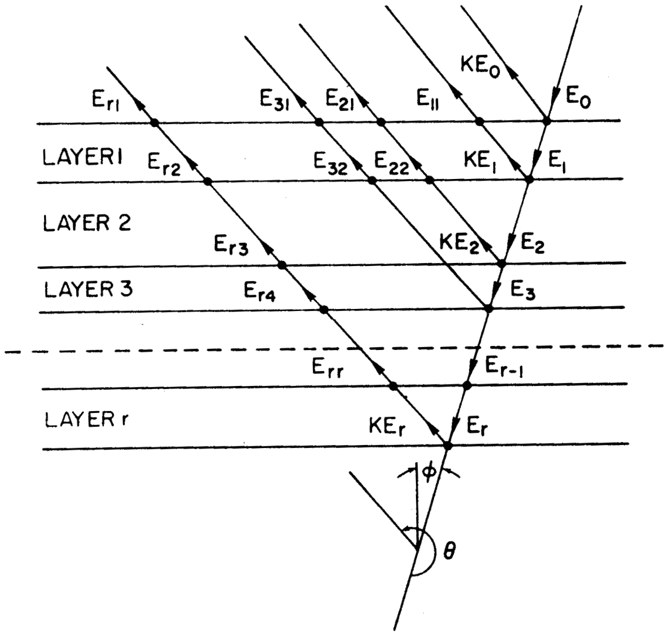
- Interactive vs. automated

- Interactive: relies on knowledge, experience and skill of user
  - time and patience limits of the user
- Automated: relies on χ^2 or similar
  - Ambiguity of data
  - χ^2 function very sensitive to the quality of the simulation
  - fully automated processes can lead to artefacts in the depth profiles derived, unless the user restricts the solution space to physical solutions
  - some form of automation is desirable, particularly if large quantities of data are to be analyzed

Types of codes

- Deterministic vs. Stochastic (Monte Carlo) (vs. ANNs)

- Deterministic
  - Fast
  - Rely on models
  - Current standard



- Monte Carlo
  - Great potential
  - Not yet ready for routine data analysis (?)

- Artificial neural networks
  - Great for large amounts of data
  - Black boxes without physics

Capabilities of codes

- Design basis
  - Techniques implemented
  - Experimental conditions supported
  - Description of samples
- Data bases implemented
  - Stopping powers
  - Scattering cross sections
- Basic physics
- Advanced physics
- Automated optimisation
- Usability

Capabilities of codes

- Basic physics

- Straight trajectories
- Single large angle scattering event
- Energy loss (e.g. SRIM)
- Flat surfaces and interfaces

- Straggling
- Screening

- RUMP and other first generation codes
- Good enough for many samples and experimental conditions
- Terribly inadequate for many other (most current problems)

Capabilities of codes

- Advanced physics and models

- Straggling with multiple scattering, geometrical straggling,…
- Non-Gaussian energy distribution
- Plural large angle scattering events (plural scattering)
- Handling of sharp resonances in the cross section
- Handling of the yield at very low energies
- Effect on yield of multiple scattering
- Rough surfaces and interfaces
- Inclusions, quantum dots, other 3D structures
- …
    - NDF and SIMNRA include several of these; MC codes
    - Room for further developments and improvements!

Capabilities of codes

➢ Design basis

Analysis Program	Incident Ions	Analytical Techniques	Scattering Geometries	Pileup correction	Detection Systems	Stopper Foils	Energy calibration
DEPTH	All	RBS, ERDA, NRA	IBM, Cornell	No	Energy dispersive (magnetic spectrograph coming)	Simulated; including inhomogeneities	Linear
GISA	All	RBS	IBM	No	Energy dispersive	N/A	Quadratic
MCERD	All	ERDA, RBS	IBM	No	Energy dispersive, TOF, different layers in detector for e.g. gas detectors	Simulated; equivalent treatment to sample	Linear
NDF	**All**	**RBS, ERDA, non-resonant NRA, PIXE, NDP, resonant NRA**	**IBM, Cornell, General**	**Yes**	**Energy dispersive**	**Simulated; equivalent treatment to sample**	**Quadratic; varying by ion species**
RBX	All	RBS, ERDA, non-resonant NRA	IBM, Cornell	Yes	Energy dispersive	Simulated; Homogeneous foils only	Linear
RUMP	**All**	**RBS, ERDA**	**Cornell, IBM, General**	**Yes**	**Energy dispersive, partial TOF**	**Simulated, or from user calibration**	**Linear**
SIMNRA	**All**	**RBS, ERDA, non-resonant NRA**	**IBM, Cornell, General**	**Yes**	**Energy dispersive, TOF, electrostatic, thin solid state detectors with transmission of particles**	**Simulated; equivalent treatment to sample**	**Quadratic; varying by ion species**

Capabilities of codes

➢ Design basis

Analysis Program	Sample Description	Continuous Profiles	Slab Limitations /Elements	Substrate Roughness	Layer Roughness
DEPTH	Layer definition	Slabs only	None	No	No
GISA	Layer definition or profile function	Maps continuous profiles onto slab structure	10 layers; 10 elements; User can define so layer*elem. is constant	No	No
MCERD					
NDF	**Layer definition; equation overlays**	**User defined functions; Effective interdiffusion profiles between layers.**	**250 layers in description; up to 92 constituents**	**Yes - approximated as energy broadening**	**Yes - approximated as energy broadening**
RBX	Layer definition	User defined functions (Gauss, error functions etc.). Channeling defect distributions.	None	No	No
RUMP	**Layer definition with equation overlays**	**Gaussian implants, error function diffusion, Pearson IV profiles, one-sided and two-sided diffusion.**	**None**	**No**	**Yes - single or dual sided, all interfaces possible.**
SIMNRA	**Layer definition**	**Slabs only**	**100 layers in description; 40 elements per layer**	**Yes - Lorentzian or Gaussian angular distribution**	**Yes, all interfaces possible.**

Capabilities of codes

➢ Physics handled

Analysis Program	Isotope Calculation	Screening Calculation	Straggling models	Plural Scattering	Multiple Scattering	Geometric Straggling	Channeling
DEPTH	Single isotope	Yes	Bohr, Chu, Yang, Tschalär	None	Yes. Pearson VII distribution	Yes	No
GISA	Natural abundance and/or specific isotopes	Energy/Angle - external tables by users	Bohr + Lindhard/Scharff	None	None	No	No
MCERD	Natural abundance and/or specific isotopes	No	Bohr, Chu, Yang	Full MC calculation	Full MC calculation	Yes	No
NDF	**Natural abundance and/or specific isotopes**	**Energy/Angle – Andersen and L'Ecuyer**	**Bohr, Chu, Yang, Tschalär**	**Dual scattering approx. (run time option)**	**Yes - Gaussian approximation from DEPTH calculation**	**Yes - from DEPTH calculation**	**No**
RBX	Natural abundance and/or specific isotopes	Yes	Bohr, Chu, Yang, Tschalär	None	Yes (same model as DEPTH)	Yes	Yes (analytic model)
RUMP	**Natural abundance and/or specific isotopes**	**Energy only - L'Ecuyer**	**Bohr**	**None**	**None**	**No**	**No**
SIMNRA	**Natural abundance and/or specific isotopes**	**Energy/Angle - Andersen and L'Ecuyer**	**Bohr, Chu, Yang, Tschalär**	**Dual scattering approx. (run time option)**	**Yes (DEPTH model approximated as Gaussian +)**	**Yes**	**No**

Capabilities of codes

➢ Fitting capabilities

Analysis Program	Starting conditions	Optimization method	Error estimation	Statistics used	Searchable experimental parameters	Auto-refinement of layers	Limitations
GISA	Reasonable guess	$\chi 2$ minimization	None returned		None	No	One layer at a time
NDF	**Elements present only; guess can be used but not required**	**Simulated annealing plus grid search**	**Bayesian inference with Markov chain Monte Carlo integration (time intensive)**	**Poisson**	E_0, E_{cal}, **charge,** θ, Φ, φ	**Yes**	**All parameters variable, user controls which ones change**
RUMP	**Reasonable guess**	**Marquart search**	**Curvature of chi-square matrix; full correlation of error sensitivities (intrinsic in search method)**	**Poisson**	E_0, E_{cal}, **charge, current,** θ, Φ, φ	**No**	**No internal limit, practical of 30 parameters at a time**
SIMNRA	**Reasonable guess**	**Simplex search**	**Additional search to determine curvature near best fit (comparable to fit time)**	**Poisson**	E_{cal}, **charge**	**No**	**One layer at a time, all characteristics**

Capabilities of codes

➢ User interface

Analysis Program	Primary Interface "nature"	Primary simulation modes	Graphic Output
DEPTH	Interactive or batch	Manual iteration	N/A
GISA	Interactive	Manual iteration; automated parameter search	Screen only
MCERD	Batch	Manual iteration	N/A
NDF	**Batch directed or interactive**	**Fully automated search; manual iteration**	**Publication quality**
RBX	Interactive	Manual iteration	Draft quality
RUMP	**Interactive**	**Manual iteration; automated parameter search**	**Publication quality**
SIMNRA	**Interactive**	**Manual iteration; automated parameter search**	**Draft quality**

Accuracy of codes and experiments

- Counting statistics
  - Often quoted as "the" error, often severely underestimates true error.
- Basic physical quantities
  - Accuracy of elastic scattering cross sections varies widely from experiment to experiment. Often strong angular dependence. Need to check original reference!
  - Stopping powers: SRIM off 4.2% and 4.1% for H and He ions on average, but for some elements errors can be much larger! For heavy ions as well: need to check original reference, and in some cases use experimental values.
- Experimental conditions
  - Error often unknown and disregarded
- Physical models and their implementations
  - For simple cases: see the IAEA intercomparison exercise
  - For complicated cases: deep knowledge is required

Effect of some phenomena on data analysis

phenomenon	*ion*	*energy*	*scattering angle*	*target element*	*effect on spectrum*	*error*	*effect on analysis*
cross section							false quantitative analysis
1) electron screening	all	all	<15º	all	decreased yield	Poorly known (large)	
	all	> 150 keV/Z	>15º	heavy		1%	
	all	> 500 keV/Z	>90º	heavy		≥0.2%	
2) nuclear effects	p	≥ 100 keV	all	light (medium heavy)	increased or decreased yield	depends on reaction (can be very large)	
	α	≥ 2.0 MeV	all	light			

Effect of some phenomena on data analysis

phenomenon	*ion*	*energy*	*scattering angle*	*target element*	*effect on spectrum*	*error*	*effect on analysis*
stopping power							false quantitative and depth analysis
1) general uncertainties	p			all	increased or decreased yields and widths	4.2% average (>10% for 13% of target atoms)	
	α			all		4.1% average (>10% for 11% of target atoms)	
	α			Si		≤2%	
	Li			all		5.1% average (>10% for 17% of target atoms)	
	heavier ions			all		6.1% average (>10% for 18% of target atoms)	
2) Bragg rule violations	all			Compounds with light elements (insulators)	increased or decreased yields and widths	≤10-15%	
3) physical state effects	all			light solids vs. liquid or gaseous	increased or decreased yields and widths	≤5-10%	

Effect of some phenomena on data analysis

phenomenon	*ion*	*energy*	*scattering angle*	*target element*	*effect on spectrum*	*error*	*effect on analysis*
energy spread, multiple scattering	heavy		grazing angle geometry		increased or decreased edge and peak broadness	large	false interdiffusion, mixing, depth profile, and roughness analysis
	p		normal incidence			small	
	all		all			depends on details (can be small or large)	
surface and interface roughness	all			all	increased edge and peak broadness, changed shape	depends on details (can be small or large)	false analysis of intermixing and interdiffusion
channeling	all		incidentally aligned geometry		decreased yields	depends on details (can be small or large)	false quantitative and depth analysis
pulse pile-up	all			heavy (all)	increased or decreased yields, background	≤2-5% for count rates below ≈5 kHz	false quantitative analysis, reduced sensitivity
low energy background	all	low (all)	grazing geometry (all)	heavy (all)	increased background	depends on the details; can be dominant at low energies; small in most analyses	false quantitative analysis, reduced sensitivity

Accuracy of codes and experiments

- Always:
  - Select a code that actually can analyse your data correctly.
  - include Andersen et al. electron screening in the calculations.
  - For proton beams, and ^{4}He beams above 2.0 MeV, always check the literature and IBANDL for possible nuclear reactions.
  - Use the most recent stopping power data available.
  - Be aware of the accuracy with which you know the exp. parameters.

Accuracy of codes and experiments

- Depending on the experiment at hand:
  - Calculate pile-up whenever count rate is not very low.
  - Calculate all contributions to energy spread whenever width of signals is relevant (e.g. diffusion, profiles, roughness). Use NDF or SIMNRA.
  - Calculate effect of roughness whenever relevant. Use NDF or SIMNRA.
  - Different codes have different emphasis and different advantages and disadvantages.

Conclusions

- Software does not replace the judgment of the analyst.
- Software that is not correctly used, or used outside its scope of application, leads to wrong data analysis.
- Use RUMP for simple RBS/ERDA, NDF and SIMNRA for best accuracy.