

Evaluation of non-Rutherford alpha elastic scattering cross-sections for silicon

Alexander F. Gurbich¹ & Chris Jeynes

University of Surrey Ion Beam Centre, Guildford, England

***¹On leave from :-
Institute of Physics & Power Engineering, Obninsk, Russia***

Acknowledgements

The **Leverhulme Trust** :- Visiting Professorship for A.F.Gurbich:
also colleagues at Surrey: **Jeff Tostevin & Ed Simpson** exploring
complementary use of SigmaCalc (Gurbich) and AZURE (Azuma++)

IAEA for supporting IBANDL and SigmaCalc
www-nds.iaea.org/ibndl & www-nds.iaea.org/sigmacalc

Engineering & Physical Sciences Research Council (**EPSRC**, UK) for
supporting the EBS measurements made in September 2005
(grant GR/R 50097)

The **Royal Society** (UK) for funding A.F.Gurbich's visit to Surrey in 2005

This work has been supported by the European Community as an
Integrating Activity «Support of Public and Industrial Research Using Ion
Beam Technology (**SPIRIT**)» under EC contract no. 227012

Contents

- Introduction – Materials Analysis
- The $^{28}\text{Si}(\alpha,\alpha)^{28}\text{Si}$ reaction
- Summary

Contents

- Introduction – Materials Analysis
 - *Surrey Ion Beam Centre*
 - Materials Modification by Ion Implantation
 - Thin Film Depth Profiling by Ion Beam Analysis
 - *Ion Beam Analysis Overview*
 - Atomic Excitation – PIXE
 - Nuclear Excitation – RBS, EBS, ERD, NRA
 - Scanning microbeam, channelling, external beam
 - *PIXE + Backscattering – self-consistent analysis*
 - *Accurate analysis!*
- The $^{28}\text{Si}(\alpha,\alpha)^{28}\text{Si}$ reaction
- Summary

Controllable Materials Modification

- **Facilities**

- *0.4-2MV High Energy Implanter (1991)*
- *2-200kV High Current Implanter (1997)*
- *Implantation 2keV \Rightarrow 4MeV (up to 10mA)*
- *Sample size $\frac{1}{4}mm^2$ to $\frac{1}{4}m^2$*
- *Hot (1000°C) or cold (~LN & 10K)*
- *Sample chambers in class 100 clean room*

- **Applications**

- *Ion Beam Synthesis*
 - Buried and surface oxides, silicides etc
- *Ion Implantation*
- *Defect Engineering*
- *Proton beam lithography (using Tandem)*
 - potentially nm resolution to 10 μ m depths



IBA equipment at Surrey

- 2 MV Tandem
 - Installed & commissioned 2002
 - up to: 4 MeV $^1\text{H}^+$; 6 MeV $^4\text{He}^{++}$; 12 MeV $^{197}\text{Au}^{5+}$
 - -ve beam injection
 - duoplasmatron source good for H^- , He^+
 - For He^- use Li vapour charge exchange
 - Nitrogen gas stripper at HV terminal
 - Pressure vessel SF_6 at 6.5 bar
- 5 beam lines
 - Microbeam (1x1 μm); nanobeam (30x30 nm ??)
 - Broad beam (100x100 μm); external beam (50x50 μm); PIGE/PINE line
 - Vertical beam line for radiation biology (500x500 nm)
 - 6-axis goniometer: 100 x 150 mm stage



Contents

- Introduction – Materials Analysis
 - *Surrey Ion Beam Centre*
 - Materials Modification by Ion Implantation
 - Thin Film Depth Profiling by Ion Beam Analysis
 - *Ion Beam Analysis Overview*
 - Atomic Excitation – PIXE
 - Nuclear Excitation – RBS, EBS, ERD, NRA
 - Scanning microbeam, channelling, external beam
 - *PIXE + Backscattering – self-consistent analysis*
 - *Accurate analysis!*
- The $^{28}\text{Si}(\alpha,\alpha)^{28}\text{Si}$ reaction
- Summary

Ion Beam Analysis Methods

RBS

Energy of scattered protons or He give light element composition and elemental depth profiles

0.2 – 4 MeV protons
or 0.2 – 6 MeV He⁺⁺
or 0.2 – 12 MeV Au⁵⁺
or 3He (or D?) etc

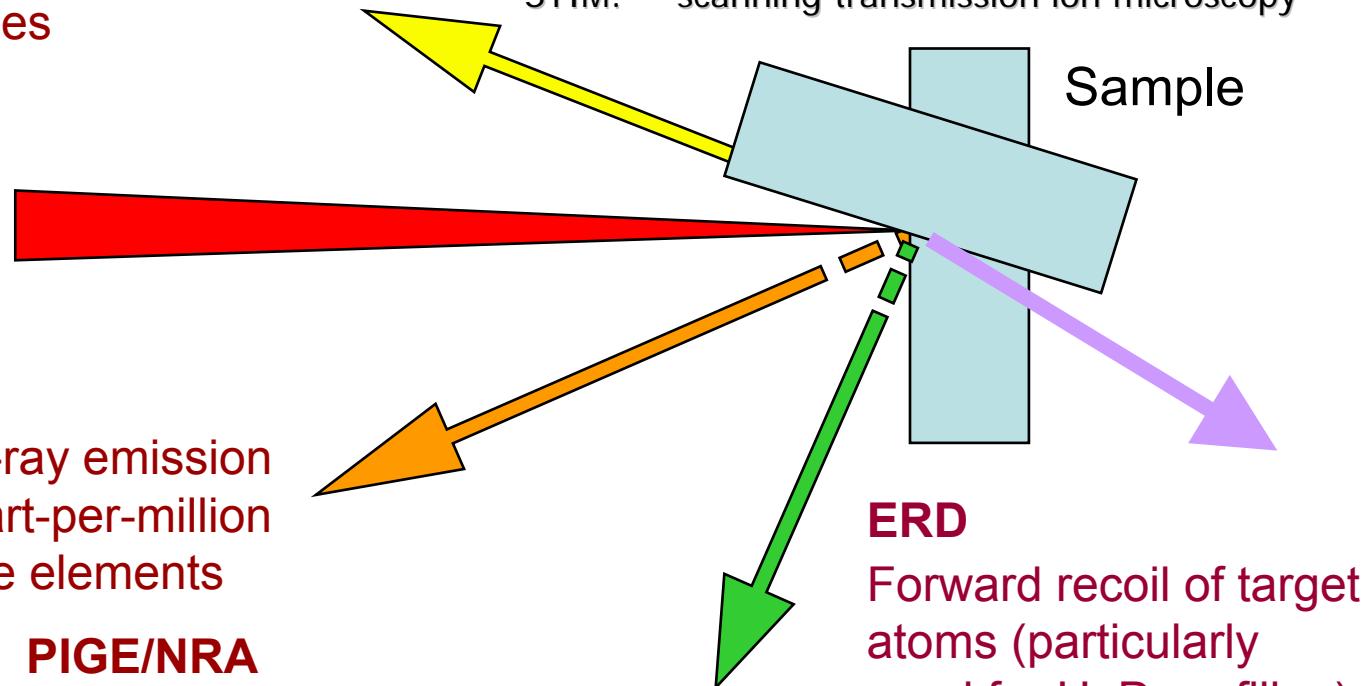
PIXE

Characteristic X-ray emission
Simultaneous part-per-million detection of trace elements from Na to U

PIGE/NRA

Nuclear reactions give characteristic gamma rays and/or particles from light nuclei (e.g. Li, B, F)

IBIL: ion beam induced luminescence
IBIC: ion beam induced current
STIM: scanning transmission ion microscopy



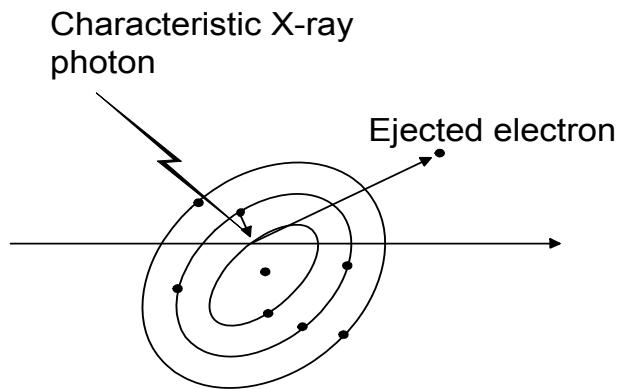
ERD

Forward recoil of target atoms (particularly good for H, D profiling)

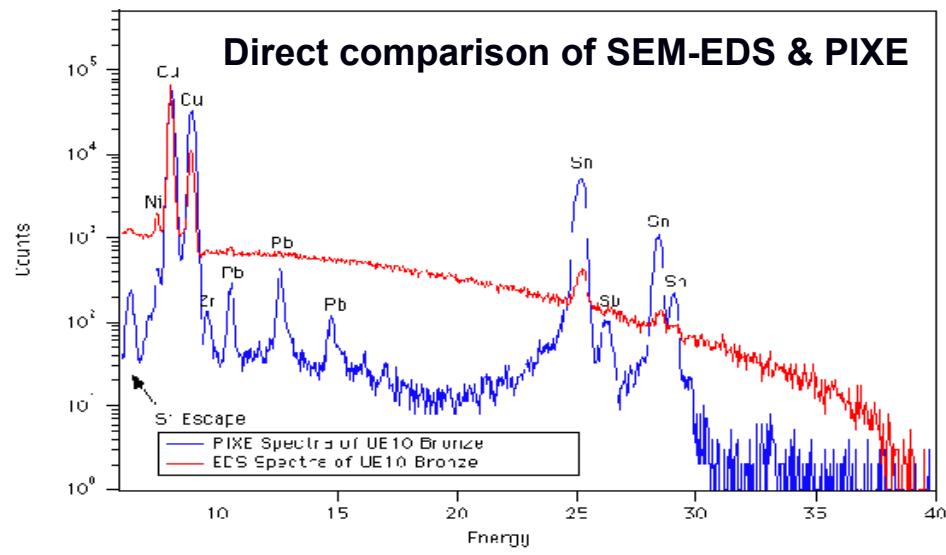
IBA Methods

- Atomic excitation
 - ***PIXE (particle-induced X-ray emission)***
 - As for SEM-EDX or EPMA (electron excitation), XRF (X-ray excitation)
 - High cross-sections relative to nuclear excitation
- Nuclear excitation
 - ***Particle elastic scattering (RBS, EBS, ERD)***
 - Rutherford scattering (Coulomb potential, point charges)
 - non-Rutherford scattering (Schrödinger's equation, elastic exit channel)
 - ***Particle nuclear reactions (NRA, PIGE)***
 - Schrödinger's equation, inelastic exit channel
 - eg. $^{27}\text{Al}(\text{p},\gamma)^{28}\text{Si}$, $^{11}\text{B}(\alpha,\text{p}_0)^{14}\text{C}$,
 - $^{15}\text{N}(\text{p},\alpha_0)^{12}\text{C}$ and $^1\text{H}(^{15}\text{N},\alpha_0)^{12}\text{C}$ are inverse reactions
 - $^{15}\text{N}(\text{p},\alpha\gamma_{1-0})^{12}\text{C}$ is the same as $^{15}\text{N}(\text{p},\alpha_1)^{12}\text{C}$ (gamma energy 4439 keV)
 - $^{14}\text{N}(\text{d},\alpha_0)^{12}\text{C}$, $^{14}\text{N}(\text{d},\alpha_1)^{12}\text{C}$, $^{14}\text{N}(\text{d},\text{p}_0)^{15}\text{N}$ are all evaluated
- Other Methods (External beam, channelling, IBIC)

Particle Induced X-ray Emission



- Analogous to EDX using MeV protons or He
- No primary electron Bremsstrahlung, so low detection limits (1-10ppm)
- Quantitative (with RBS)
- Imaging resolution determined by beam size (*not* beam energy as in EDX)
- Very high cross-sections, so information is from femtograms of material



Johansson and Campbell, *PIXE*, Wiley 1995

PIXE

- **Sensitivity**
- **Scattering**
- **Backscattered particles**

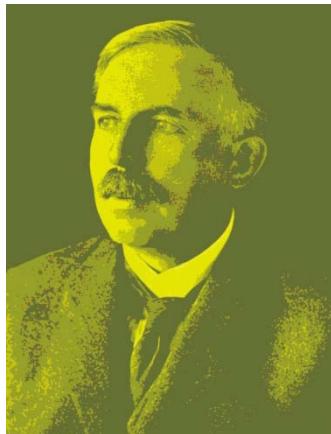
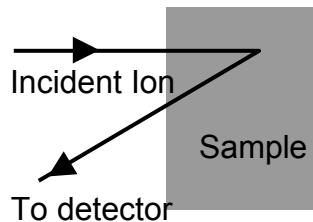
SEM-EDS and PIXE spectra for a bulk bronze sample

IBA Methods

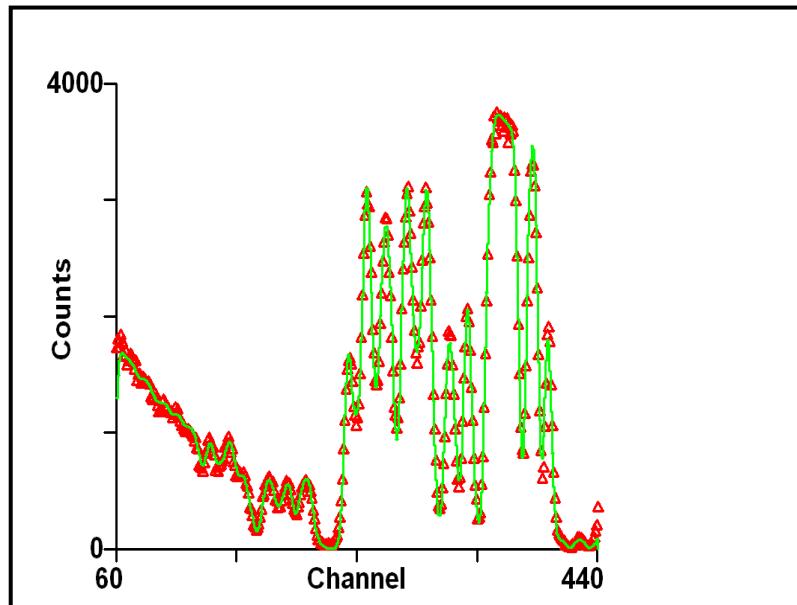
- Atomic excitation
 - ***PIXE (particle-induced X-ray emission)***
 - As for SEM-EDX or EPMA (electron excitation), or XRF (X-ray excitation)
 - High cross-sections relative to nuclear excitation
- Nuclear excitation
 - ***Particle elastic scattering (RBS, EBS, ERD)***
 - Rutherford scattering (Coulomb potential, point charges)
 - non-Rutherford scattering (Schrödinger's equation, elastic exit channel)
 - ***Particle nuclear reactions (NRA, PIGE)***
 - Schrödinger's equation, inelastic exit channel
 - eg. $^{27}\text{Al}(\text{p},\gamma)^{28}\text{Si}$, $^{11}\text{B}(\alpha,\text{p}_0)^{14}\text{C}$,
 - $^{15}\text{N}(\text{p},\alpha_0)^{12}\text{C}$ and $^1\text{H}(^{15}\text{N},\alpha_0)^{12}\text{C}$ are inverse reactions
 - $^{15}\text{N}(\text{p},\alpha\gamma_{1-0})^{12}\text{C}$ is the same as $^{15}\text{N}(\text{p},\alpha_1)^{12}\text{C}$ (gamma energy 4439 keV)
 - $^{14}\text{N}(\text{d},\alpha_0)^{12}\text{C}$, $^{14}\text{N}(\text{d},\alpha_1)^{12}\text{C}$, $^{14}\text{N}(\text{d},\text{p}_0)^{15}\text{N}$ are all evaluated
- Other Methods (External beam, channelling, IBIC)

Rutherford BackScattering

RBS



- Energy of ions scattering from nuclear collisions depends on mass and depth
- Detection limit around 0.1%
- Depth profiling with depth resolution <20nm
- Analytical cross-section σ (Coulomb potential)
- Single scattering (cf electron backscatters in SEM)



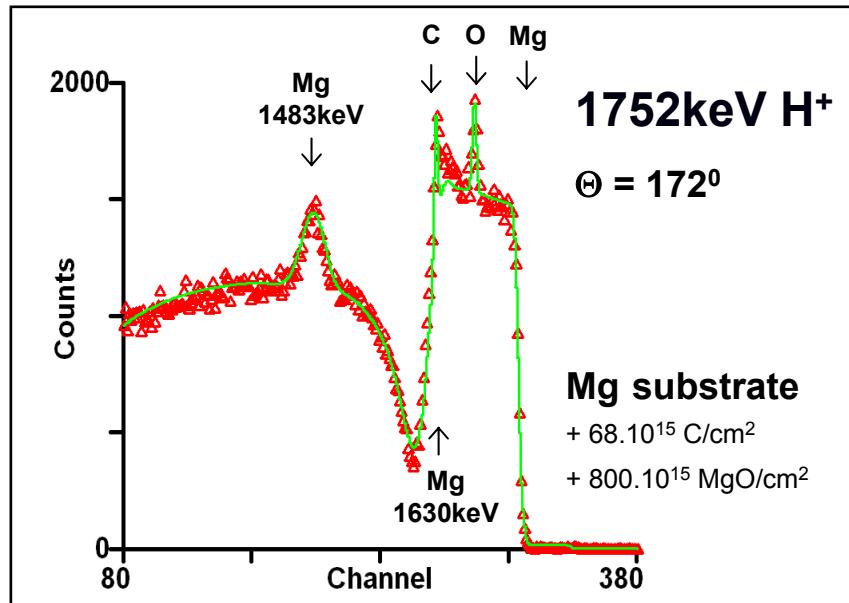
$$\sigma \text{ proportional to } Z^2/E^2$$

- Coulomb potential (accurate)
- Perfect fitting of complex structures (inverse problem solved)

Spectrum of zirconia/silica multilayer optical coating (red), with DataFurnace fit (green)

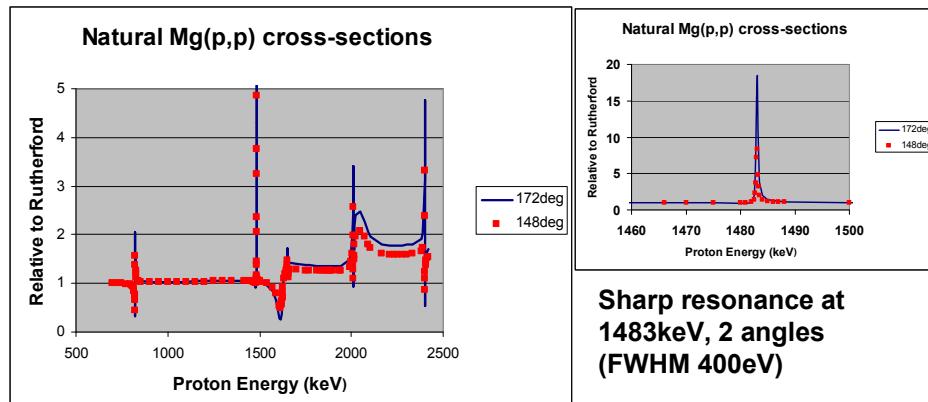
C.Jeynes++ *Surface & Interface Analysis* 30 (2000) 237-242

Elastic (non-Rutherford) BackScattering



Benchmark experiment for evaluated Mg cross-sections

Gurbich & Jeynes, Nucl.Instrum.Methods B265 (2007) 447-452



SigmaCalc scattering cross-sections for natural Mg (the isotopes behave differently) at two different scattering angles

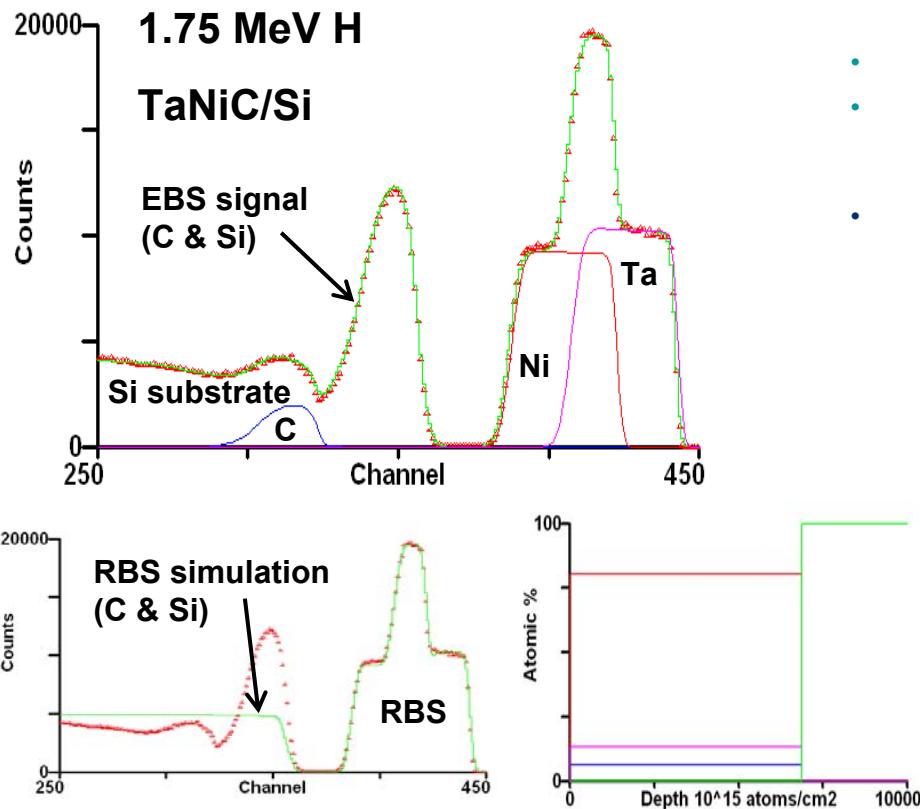
EBS

- Kinematics the same as for RBS
 - Scattering cross-sections not Coulomb
 - Can be fitted by solving Schrödinger's equation
 - See **SigmaCalc** at www-nds.iaea.org/ibandl
- Gurbich, NIM B268 (2010) 1703**
- *Greatly enhanced* cross-sections often available for light elements
 - Cross-sections vary strongly with scattering angle

For sharp resonances one must correctly calculate energy straggling in depth (this effect can be LARGE)

Barradas et al, NIM B247 (2006) 381

Elastic (non-Rutherford) BackScattering



- Cross-sections **not analytical** and must be measured
- Light elements in heavy matrix can be measured (in this case 6.6at% C in TaNiC on a silicon background signal)
- Very large cross-section enhancements, depending on target atom and beam energy

EBS spectrum of 750nm TaNiC sputtered film on Si substrate

The Ta & Ni signals are Rutherford, but the C & Si signals are strongly non-Rutherford.

Above: data & fit with Ta, Ni, C partial spectra shown

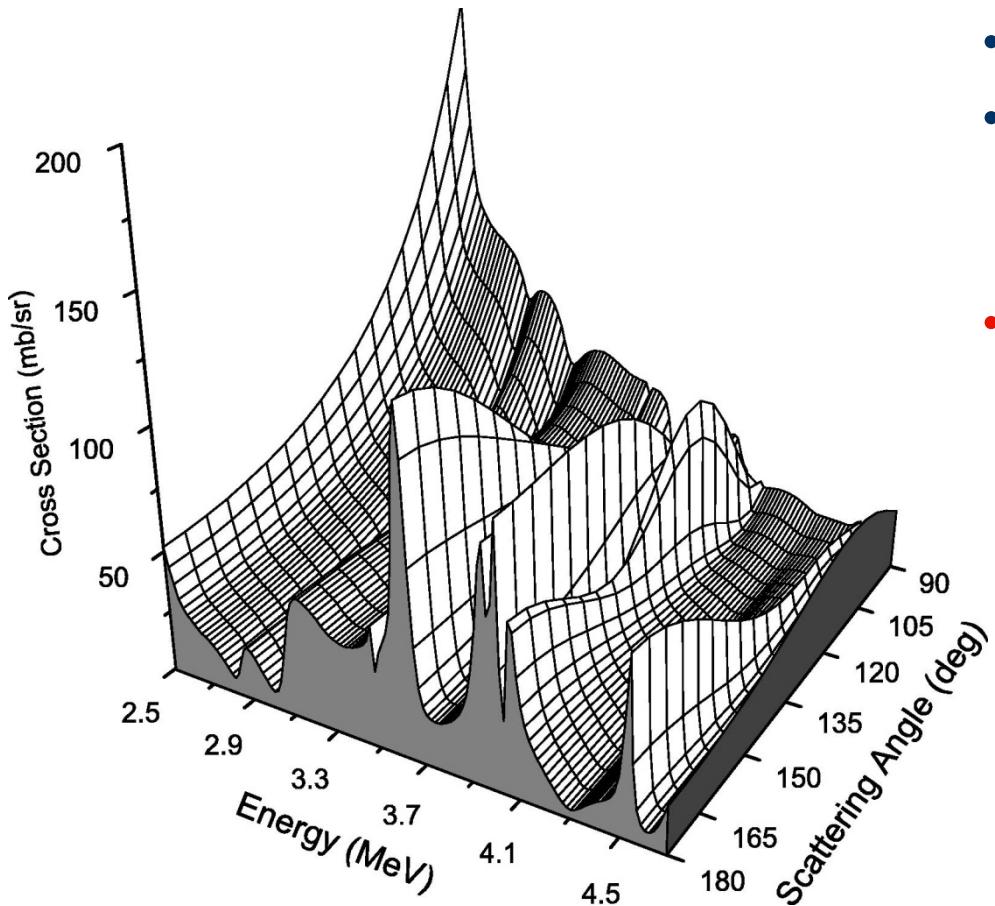
Below: simulation with RBS for Si & C

Right: Depth profile obtained

Jeynes *et al*, NIM B161-163 (2000) 287

EBS

Elastic (non-Rutherford) BackScattering



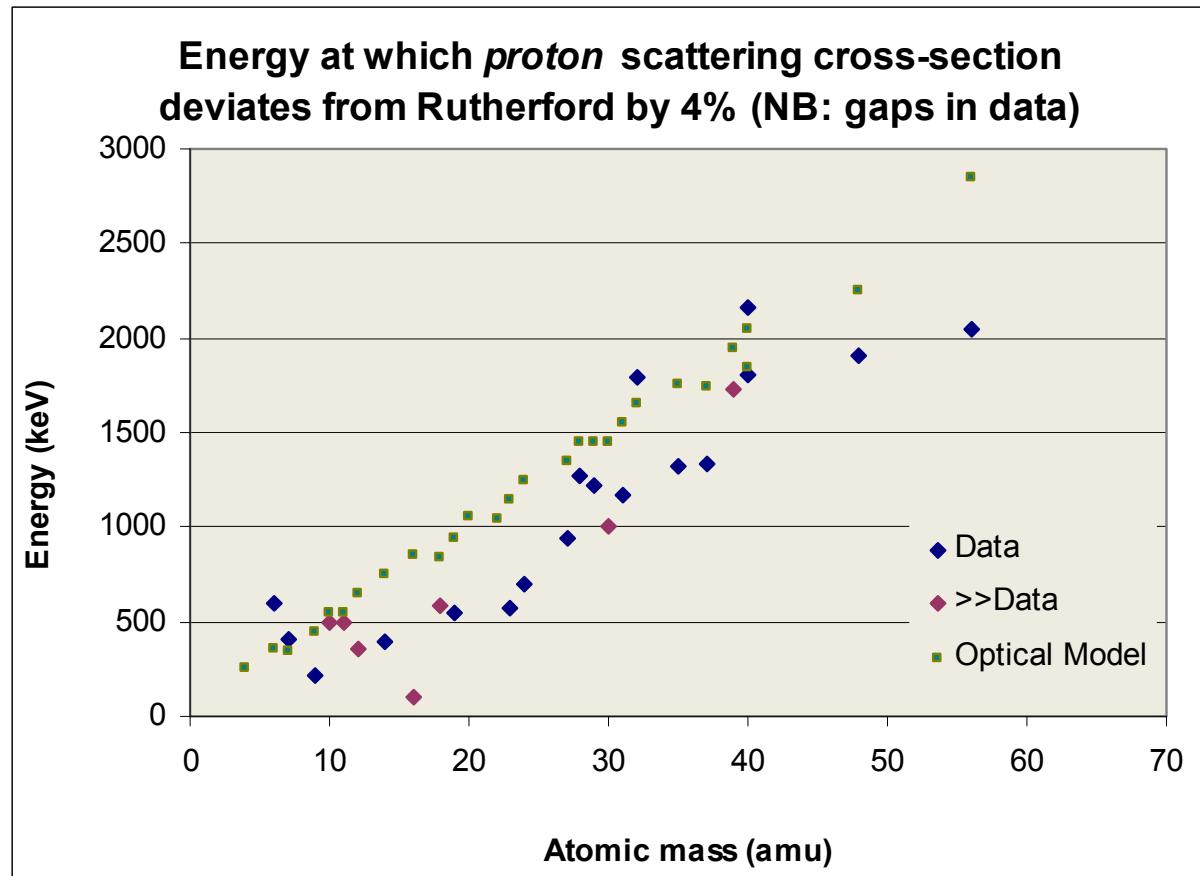
- $^{14}\text{N}(\alpha,\alpha)^{14}\text{N}$
- Variation of scattering cross-section function with scattering angle
- **Evaluated** by fitting nuclear data (including measured scattering cross-sections and gamma spectroscopy etc)

A.F.Gurbich et al, *Nucl. Instrum. Methods B*, 269 (2011) 40

See SigmaCalc at www-nds.iaea.org/ibandl

EBS

Elastic (non-Rutherford) BackScattering



From Table 1 in Jeynes, Webb & Lohstroh, *Reviews of Accelerator Science and Technology*, 4 (2011) 41–82

NB:

For 2 MeV protons cross-sections are **EBS** right up to Fe!

Notes:

“>>Data” (red): data not available for these nuclei, but boundary known to be (much) lower than point shown.

“Optical Model”: semi-classical quantum mechanics calculation

EBS

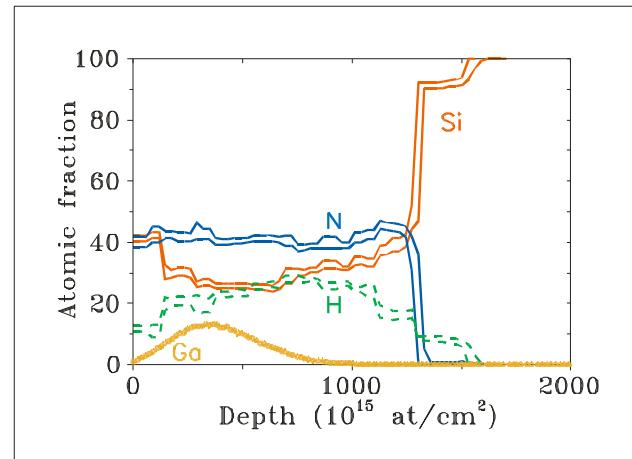
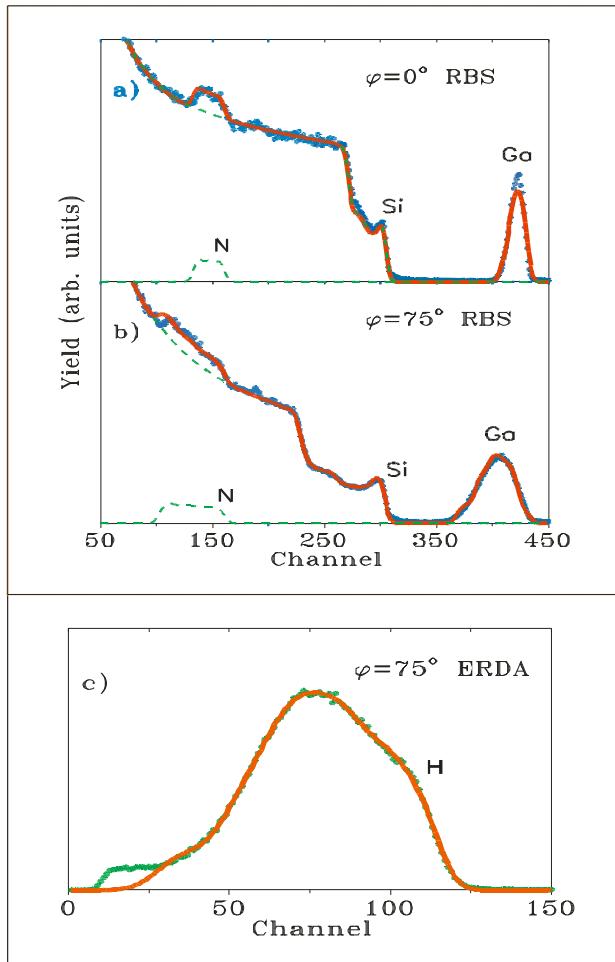
Elastic Recoil Detection

1.5MeV ${}^4\text{He}$ RBS
Normal incidence

Glancing incidence

Simultaneous with:
ERD

ERD

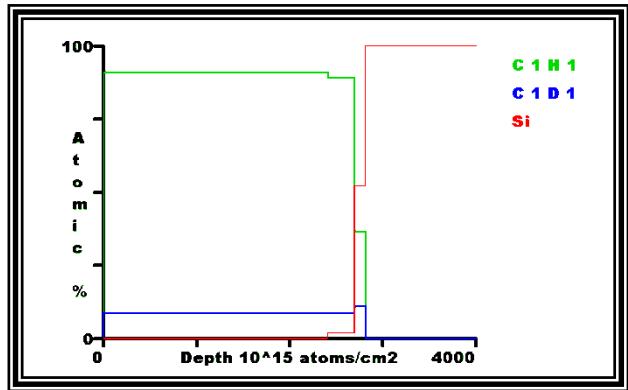


$\text{SiN}_x:\text{H}$ on Si
Ga implant to form a- GaN_x ?
Barradas *et al*, NIM B148, 1999, 463

IBA Methods

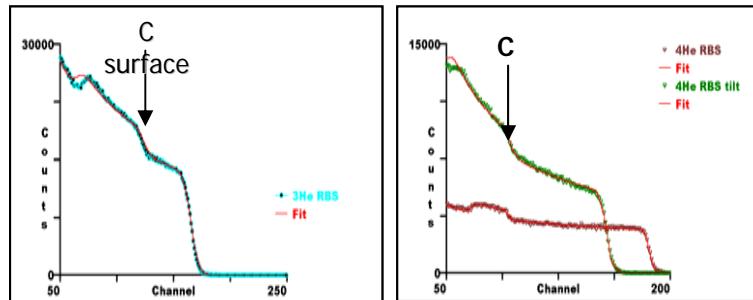
- Atomic excitation
 - ***PIXE (particle-induced X-ray emission)***
 - As for SEM-EDX or EPMA (electron excitation), XRF (X-ray excitation)
 - High cross-sections relative to nuclear excitation
- Nuclear excitation
 - ***Particle elastic scattering (RBS, EBS, ERD)***
 - Rutherford scattering (Coulomb potential, point charges)
 - non-Rutherford scattering (Schrödinger's equation, elastic exit channel)
 - ***Particle nuclear reactions (NRA, PIGE)***
 - Schrödinger's equation, inelastic exit channel
 - eg. $^{27}\text{Al}(\text{p},\gamma)^{28}\text{Si}$, $^{11}\text{B}(\alpha,\text{p}_0)^{14}\text{C}$,
 - $^{15}\text{N}(\text{p},\alpha_0)^{12}\text{C}$ and $^1\text{H}(^{15}\text{N},\alpha_0)^{12}\text{C}$ are inverse reactions
 - $^{15}\text{N}(\text{p},\alpha\gamma_{1-0})^{12}\text{C}$ is the same as $^{15}\text{N}(\text{p},\alpha_1)^{12}\text{C}$ (gamma energy 4439 keV)
 - $^{14}\text{N}(\text{d},\alpha_0)^{12}\text{C}$, $^{14}\text{N}(\text{d},\alpha_1)^{12}\text{C}$, $^{14}\text{N}(\text{d},\text{p}_0)^{15}\text{N}$ are all evaluated
- Other Methods (External beam, channelling, IBIC)

Nuclear Reaction Analysis

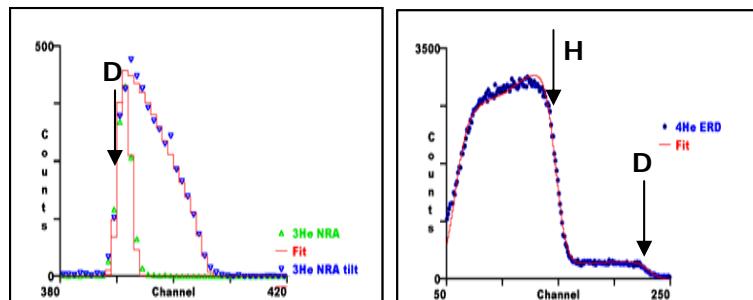


Depth profiling of 300nm CH:DH film on Si using simultaneous RBS/NRA/ERD and automatic spectrum inversion with **DataFurnace** software (Jeynes et al J.Phys.D 36, 2003, R97)

0.7MeV ^3He RBS
Normal



0.7MeV ^3He NRA
 $d(^3\text{He}, p)^4\text{He}$
 $Q=18.35\text{MeV}$
Normal & glancing

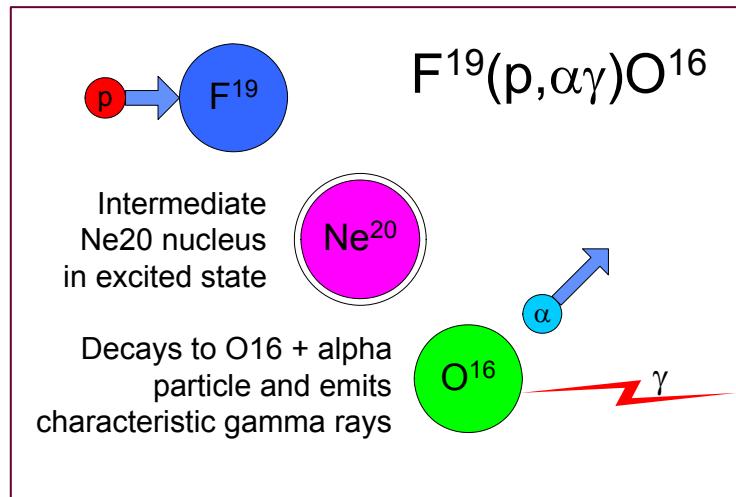


1.5MeV ^4He RBS
Normal & glancing

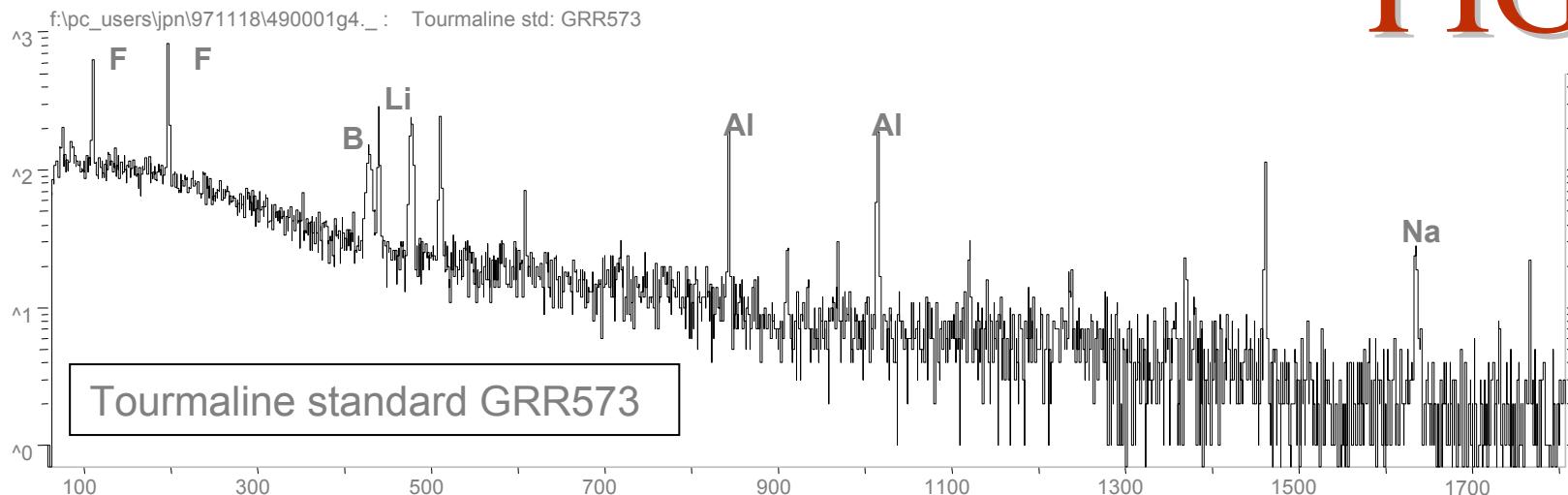
1.5MeV ^4He ERD
Glancing

NRA

Proton Induced Gamma Ray Emission

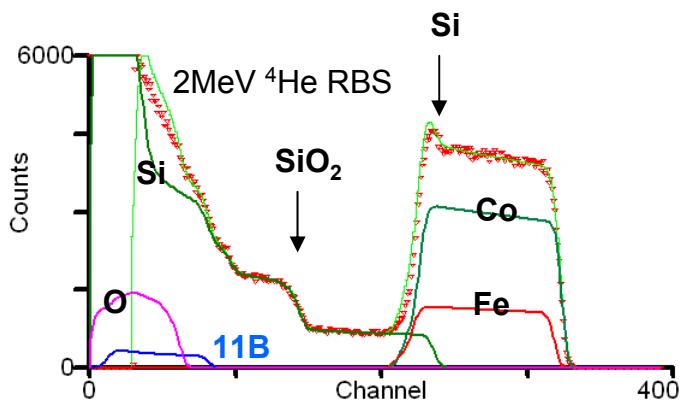


- MeV protons can overcome the Coulomb barrier of light nuclei to induce gamma emitting nuclear reactions
- Gamma energy is characteristic of specific isotopes
- Detection limits ~ 0.1 at%
- Useful for specific problems (e.g. ^{19}F , ^{11}B , ^{23}Na , ^{24}Mg , ^{27}Al)
- **Special case of NRA**

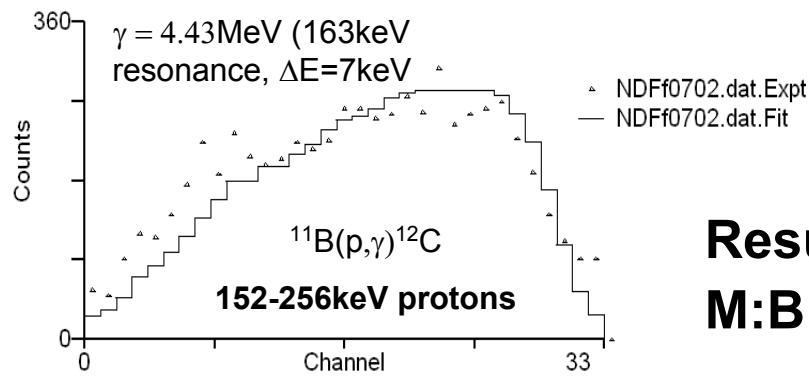


PIGE

NRP (PIGE) of metal boro-silicide sample



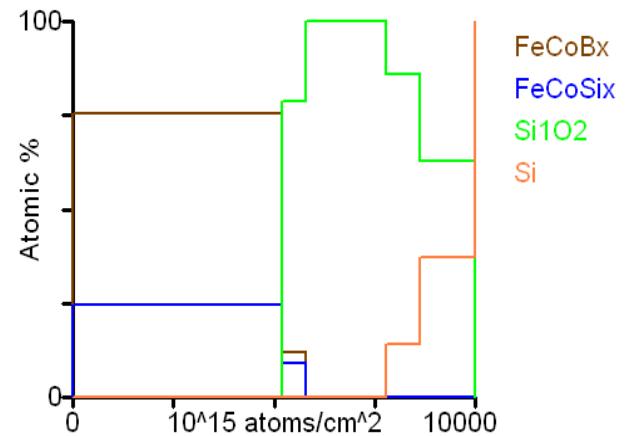
- Sample structure from **RBS** (boron content poorly determined)
- Co/Fe=3.8 from 2.2MeV **PIXE**
- *Direct PIGE signal for B with a proton beam scanned 0.1-0.3 MeV*



Result is:
M:B:Si = 26:58:16

DataFurnace integrates RBS/PIXE/PIGE for self-consistent analysis

Barradas *et al*, Nucl. Instrum. Methods B, 268 (2010) 1829–1832

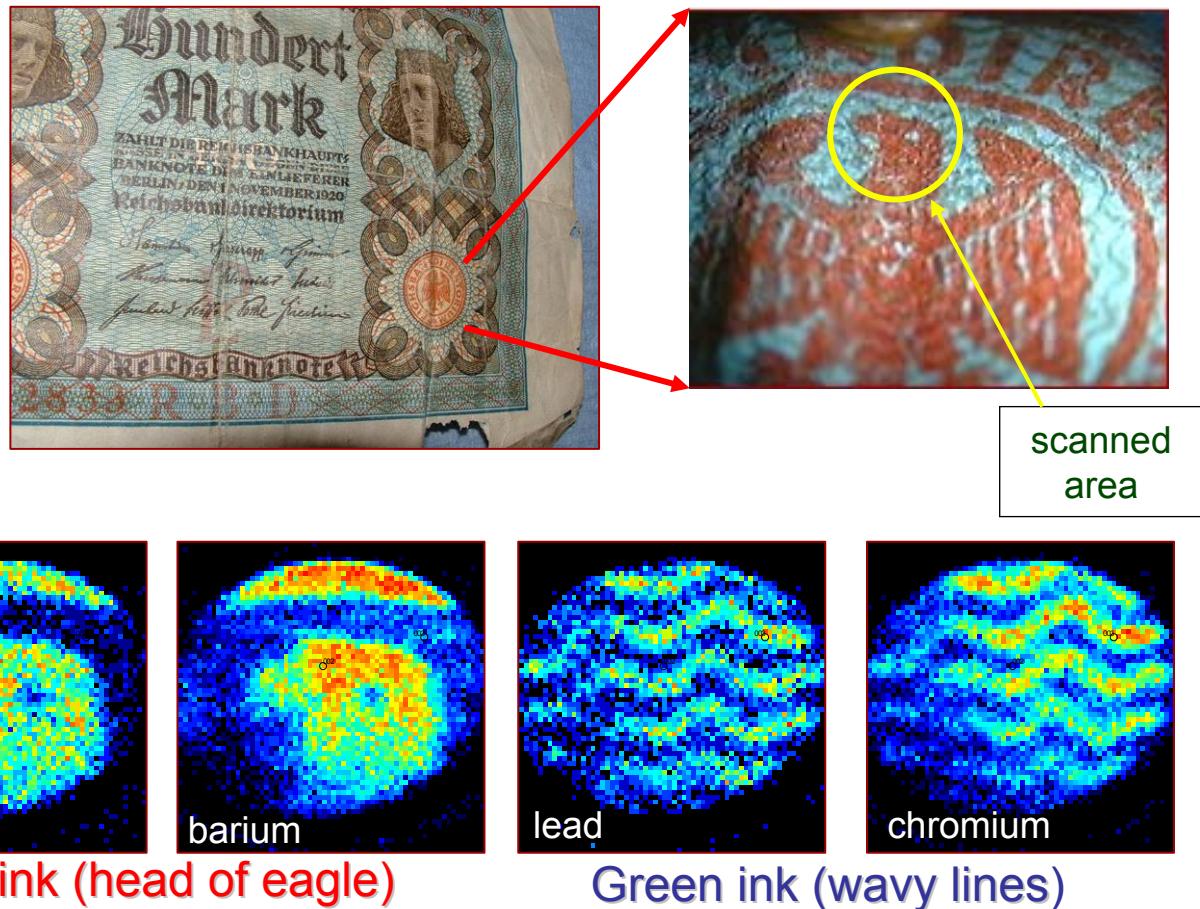


IBA Methods

- Atomic excitation
 - ***PIXE (particle-induced X-ray emission)***
 - As for SEM-EDX or EPMA (electron excitation), XRF (X-ray excitation)
 - High cross-sections relative to nuclear excitation
- Nuclear excitation
 - ***Particle elastic scattering (RBS, EBS, ERD)***
 - Rutherford scattering (Coulomb potential, point charges)
 - non-Rutherford scattering (Schrödinger's equation, elastic exit channel)
 - Accurate analysis!
 - ***Particle nuclear reactions (NRA, PIGE)***
 - Schrödinger's equation, inelastic exit channel
 - eg. $^{27}\text{Al}(\text{p},\gamma)^{28}\text{Si}$, $^{11}\text{B}(\alpha,\text{p}_0)^{14}\text{C}$,
 - $^{15}\text{N}(\text{p},\alpha_0)^{12}\text{C}$ and $^1\text{H}(^{15}\text{N},\alpha_0)^{12}\text{C}$ are inverse reactions
 - $^{15}\text{N}(\text{p},\alpha\gamma_{1-0})^{12}\text{C}$ is the same as $^{15}\text{N}(\text{p},\alpha_1)^{12}\text{C}$ (gamma energy 4439 keV)
 - $^{14}\text{N}(\text{d},\alpha_0)^{12}\text{C}$, $^{14}\text{N}(\text{d},\alpha_1)^{12}\text{C}$, $^{14}\text{N}(\text{d},\text{p}_0)^{15}\text{N}$ are all evaluated
- Other Methods (External beam, channelling, IBIC)

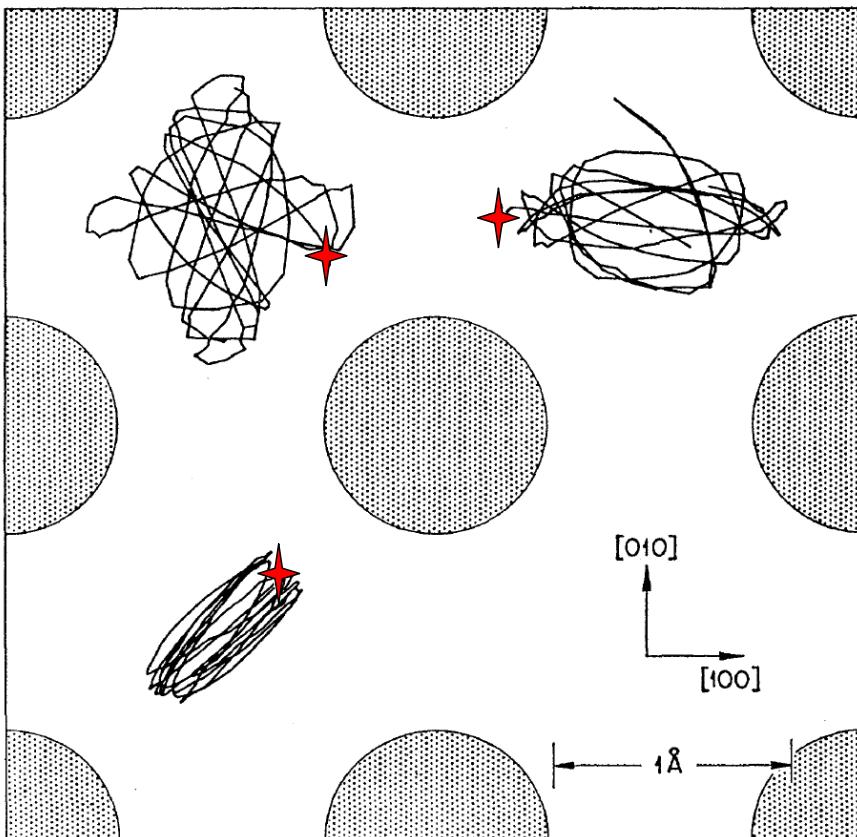
External Beam

- 100 Reichmark bank note from Germany dated 1920
- Can we analyse the inks?



10 other elements detected
Analysis carried out in 10 minutes with no visible marking of the paper

Channelling



Projection of three calculated trajectories of 1 keV Cu incident (at points marked with stars) along the (001) direction of a face centred cubic Cu crystal. The trajectories for 250 collisions are shown and the truncated Bohr potential is used.

Range in channelling can be up to 25 times “random” range

Robinson & Oen, Phys. Rev, 132 (1963) 2385

Channelling - crystalline damage example

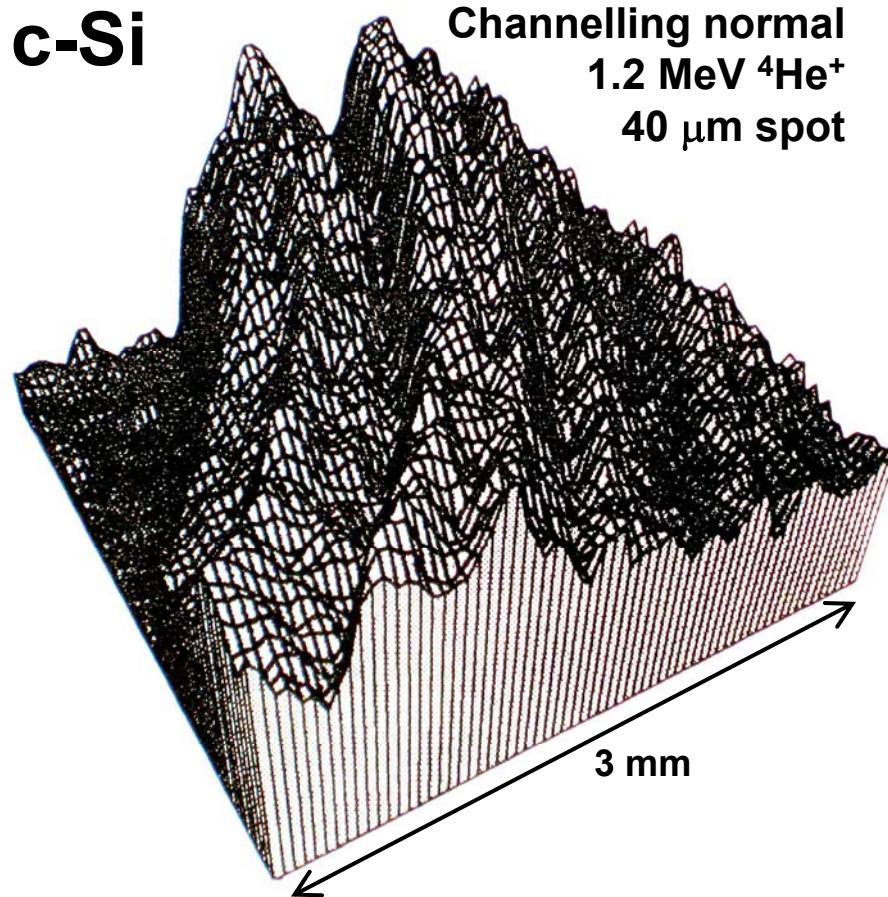


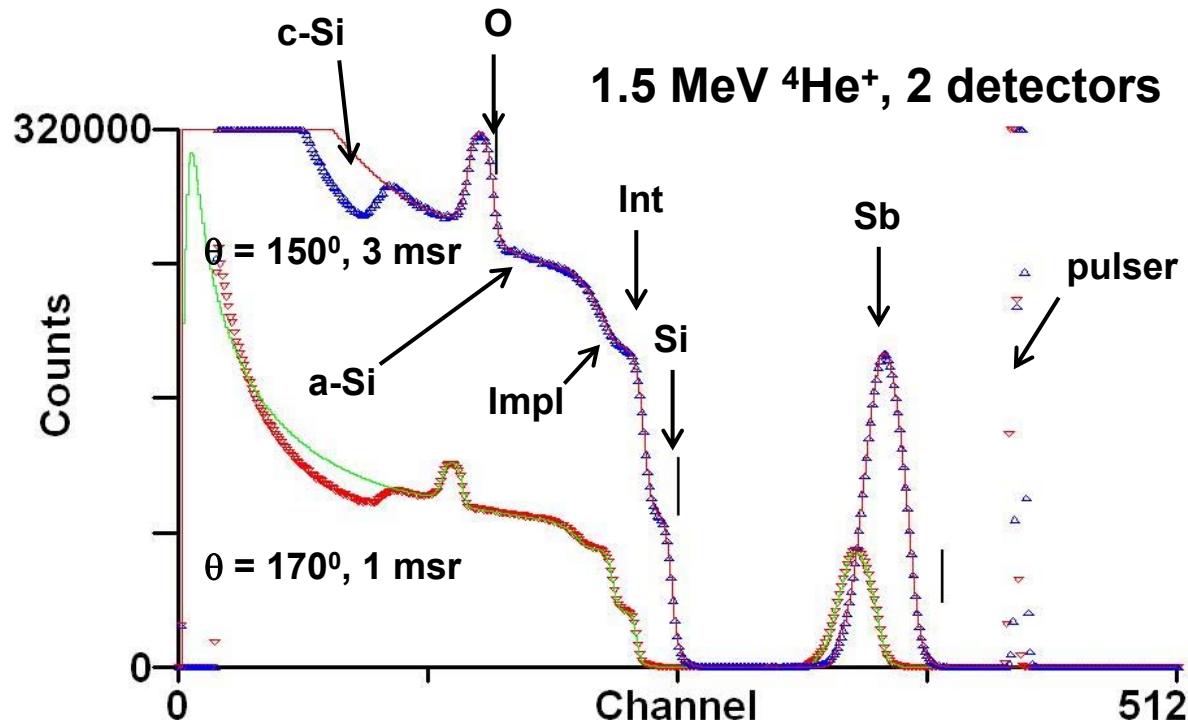
Image of circular damage tracks in a silicon sample turned on an ultra-stiff lathe with a **single-point diamond tool**.

Signal is the low-energy part of the RBS Si signal: high yield means high damage. 128×128 pixels, pixel area $(23.4 \mu\text{m})^2$, 0.15 nC/pixel.

This is **plastic** deformation of a **brittle** material, with an a-Si layer up to 350 nm thick over a **dislocation array** $\sim 5 \cdot 10^{10}/\text{cm}^2$.

Jeynes, Puttick, Gärtner et al,
Nucl. Instrum. Methods B, 118 (1996) 431

Channelling



$481.10^{14} \text{ Sb/cm}^2$ certified standard implant
Amorphised to 630 nm, 90 nm surface oxide

Barradas *et al*, *Nucl. Instrum. Meth. B*, 266 (2008) 1198-1202

The He beam is normal to the sample, channelled in the (100) direction.

The Si and O edges are marked.

The pulser and the Sb implant peaks are marked

The SiO_2/Si interface signal is marked “Int”

The energy loss in the Sb gives a dip in the Si signal, marked “Impl”

The interface between the a-Si and c-Si is clear.

Contents

- Introduction – Materials Analysis
 - *Surrey Ion Beam Centre*
 - Materials Modification by Ion Implantation
 - Thin Film Depth Profiling by Ion Beam Analysis
 - *Ion Beam Analysis Overview*
 - Atomic Excitation – PIXE
 - Nuclear Excitation – RBS, EBS, ERD, NRA
 - Scanning microbeam, channelling, external beam
 - ***PIXE + Backscattering – self-consistent analysis***
 - ***Accurate analysis!***
- The $^{28}\text{Si}(\alpha,\alpha)^{28}\text{Si}$ reaction
- Summary

Towards truly simultaneous PIXE and RBS analysis of layered objects in cultural heritage



C. Pascual-Izarra (**Madrid**), N. P. Barradas, M. A. Reis (**Lisbon**),
C. Jeynes (**Surrey**), M. Menu, B. Lavdrine, J. J. Ezrati, S. Röhrs (**Louvre**)

Nucl. Instrum. Methods B261, 426-429 (2007)

3 MeV H PIXE

3 MeV H EBS

3 MeV He RBS

Fitted depth
profile

Niepce's first Heliography:
Paysage à Saint-Loup de Varennes (1827)

Corrosion products demonstrated
by PIXE/RBS/EBS to be tin oxide in
a tin/lead matrix

Characterization of paint layers by simultaneous self-consistent fitting of RBS/PIXE spectra using simulated annealing

L. Beck (**Louvre**), C. Jeynes (**Surrey**), N.P.Barradas (**Lisbon**)

Nucl. Instrum. Methods B266, 1871-1874 (2008)

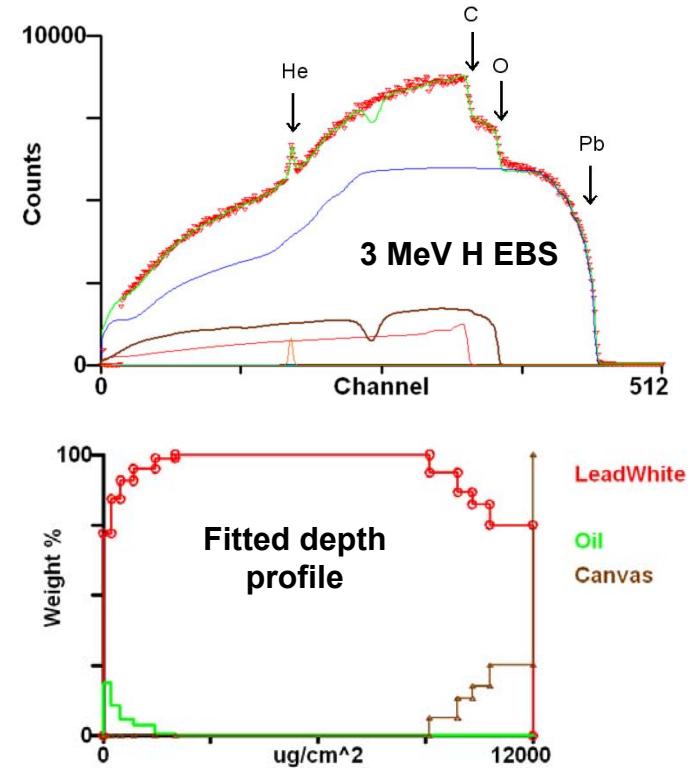


"La Bohémienne", Frans Hals 1630

AGLAЕ : Accélérateur Grand Louvre d'Analyse Élémentaire

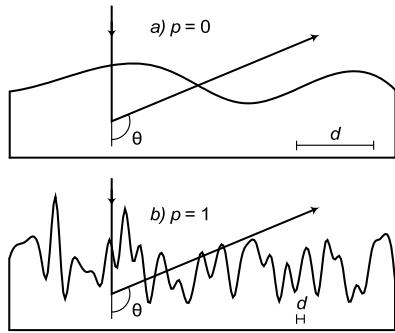


Ochre (haematite) pigment located and quantified by PIXE/RBS/EBS



Roughness

Molodtsov, Gurbich & Jeynes, J.Phys. D: Appl. Phys. 41, 205303 (2008) (7pp)

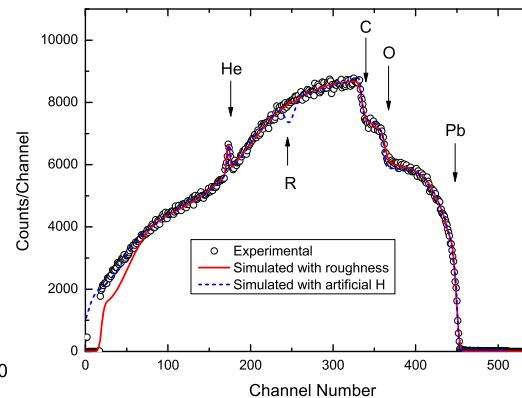
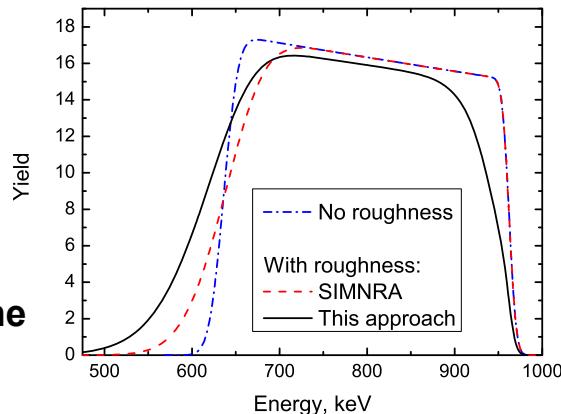


- Beam re-entering through surface asperities gives extra surface energy loss due to extra pathlength x
- Generate a general rough surface giving a pathlength density function $f(x)$
- Characterise roughness with TWO PARAMETERS: “sharpness” σ and “scale” p
- Parameterise $f(x)$ explicitly using extensive Monte Carlo calculations

$$f(x) = (1-n)\delta(x) + n \frac{b^{a+1}}{\Gamma(a+1)} x^a \exp(-bx)$$

**SIMNRA (and NDF)
can simulate only
some of the
roughness effect**

**New algorithm
calculates the high
energy effect and the
lower max yield**



**New algorithm
correctly calculates
the smearing of the
EBS resonances “R”.**

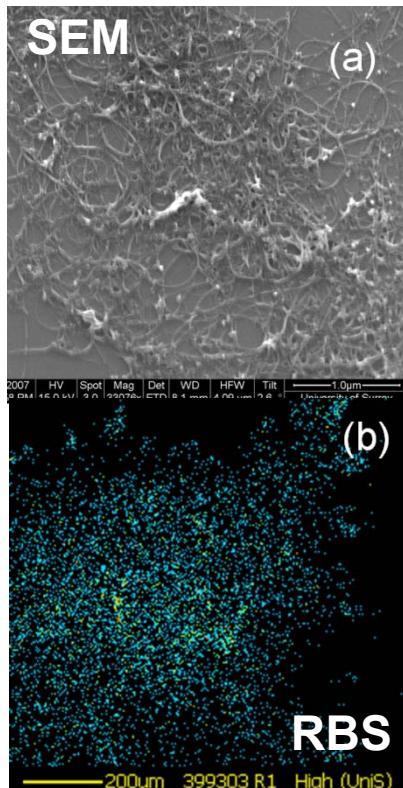
**The effect on the
depth profiles is
LARGE**

- Most real samples are ROUGH!
- Extract scale and sharpness from BS spectra without MonteCarlo
- Valid for RBS, EBS, ERD, PIXE, NRA
- Correct depth profiles!

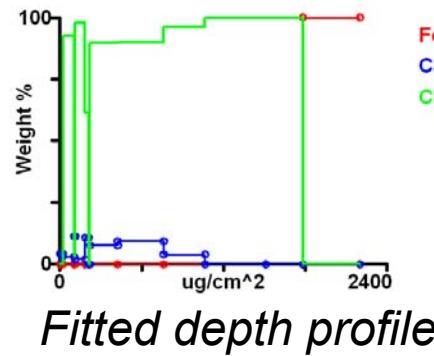
RBS/EBS/PIXE measurement of single-walled carbon nanotube modification by nitric acid purification treatment

J.C.G. Jeynes, C. Jeynes, K.J. Kirkby, M. Rümmeli, S.R.P. Silva

Nucl. Instrum. Methods B266, 1569-1573 (2008)



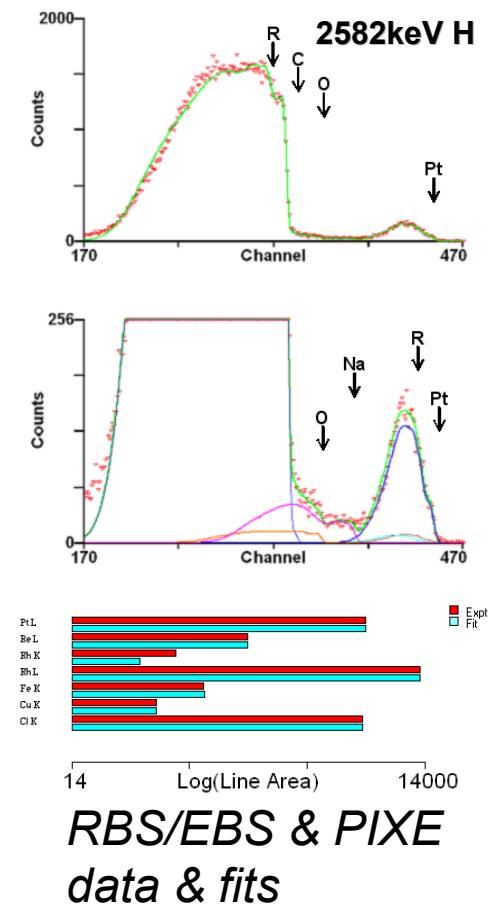
SWCNT on mylar



Fitted depth profile

O quantified by PIXE/RBS/EBS in the presence of mixed heavy metal **catalyst** content of CNT with heavy roughness

Catalyst contains Pt, Rh, Re, Fe, Cu, Cl, Na. Roughness effects marked "R"



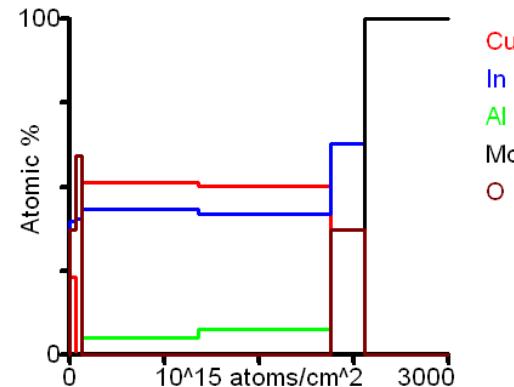
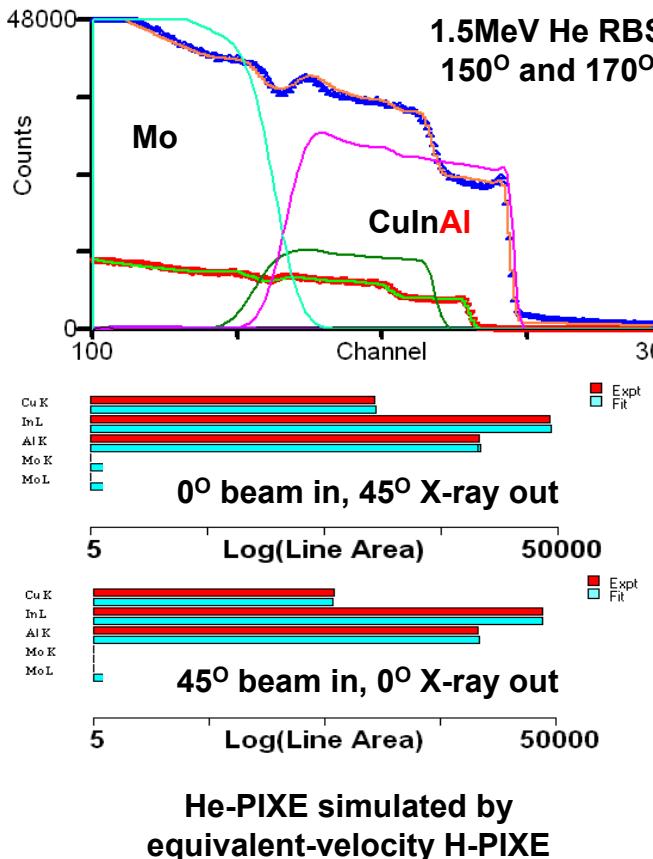
RBS/EBS & PIXE data & fits

Characterisation of thin film chalcogenide PV materials using MeV ion beam analysis

Chris Jeynes, G.Zoppi, I.Forbes, M.J.Bailey, N.Peng

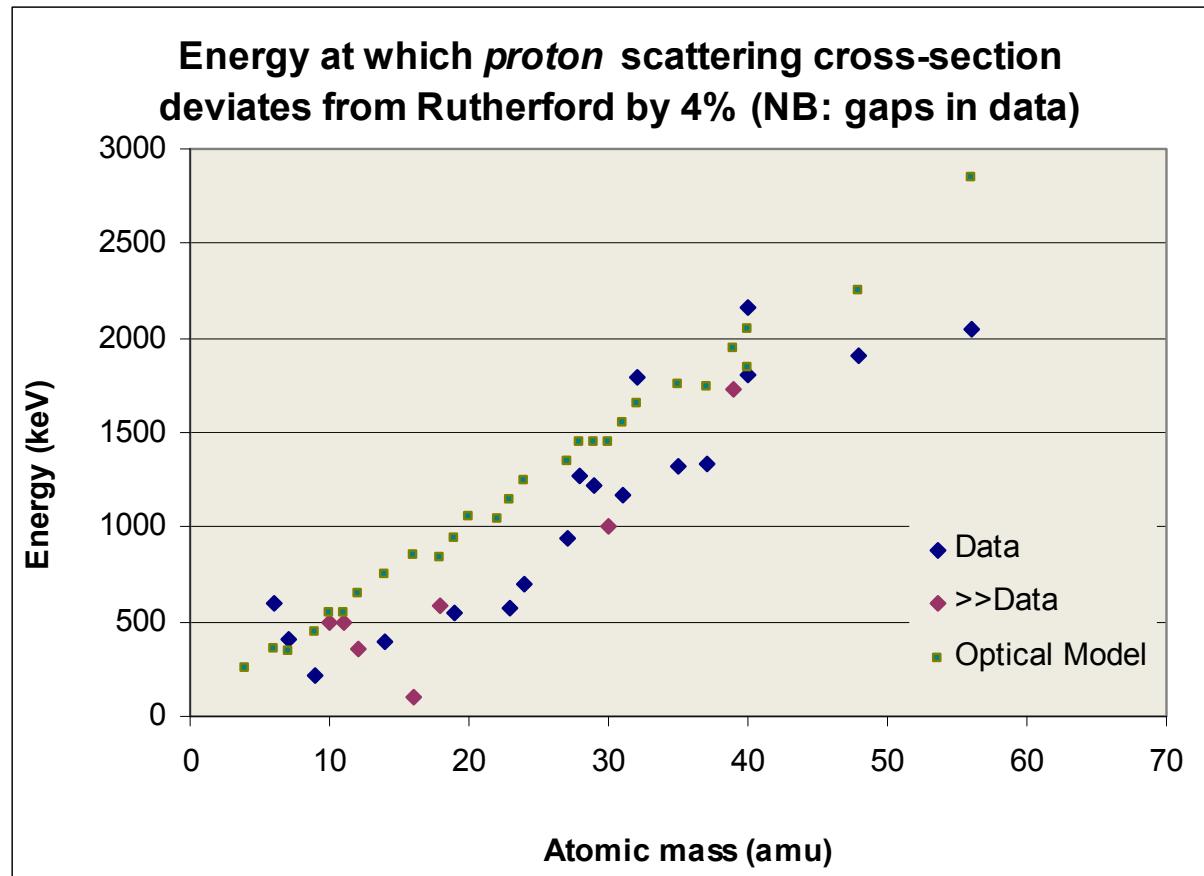
IEEE Proceedings of Supergen Conference, Nanjing,

April 2009, DOI:10.1109/SUPERGEN.2009.5348162



- CIAS semiconductor on Mo electrode
 - Precursor material (not selenided yet)
 - Al **invisible** in backscattering
 - Strong layering: PIXE **uninterpretable** without profile independently available
 - **Differential PIXE** to profile Al
 - Essential to fit roughness (**non-uniform thickness**) to reproduce RBS spectra
 - Good fit **essential** for reliable profile

Elastic (non-Rutherford) BackScattering



From Table 1 in Jeynes, Webb & Lohstroh, *Reviews of Accelerator Science and Technology*, 4 (2011) 41–82

NB:

For 2 MeV protons cross-sections are **EBS** right up to Fe!

Notes:

“>>Data” (red): data not available for these nuclei, but boundary known to be (much) lower than point shown.

“Optical Model”: semi-classical quantum mechanics calculation

EBS

Information in BS spectra with few counts

N.P.Barradas, C. Jeynes, M. Jenkin, P.K. Marriott

Thin Solid Films 343-344 (1999) 31-34

1.5 MeV He RBS

- **PIXE cross-sections >> RBS**
- **100 pA common for PIXE**
- **Poor statistics in particle spectra!**

This **Bayesian analysis** demonstrates that even spectra with very small collected charge have lots of information!

*Don't throw away good data!
Always do BS with PIXE!
Always do PIXE with BS!*

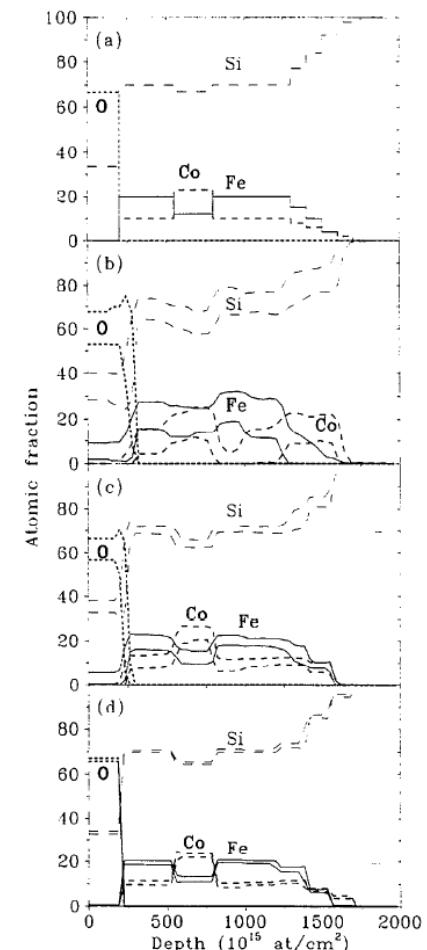


Fig. 1. (a) Theoretical depth profile used to generate the test RBS spectra analysed, with (b) high, (c) medium, and (d) low level of noise. Confidence limits (± 1 standard deviation) of the posterior probability distribution obtained with MCMC for the different elements. Oxygen was only allowed to exist at the surface of the sample, and Co and Fe were restricted to depths below 2×10^{15} at/cm².

Contents

- Introduction – Materials Analysis
 - *Surrey Ion Beam Centre*
 - Materials Modification by Ion Implantation
 - Thin Film Depth Profiling by Ion Beam Analysis
 - *Ion Beam Analysis Overview*
 - Atomic Excitation – PIXE
 - Nuclear Excitation – RBS, EBS, ERD, NRA
 - Scanning microbeam, channelling, external beam
 - Accurate analysis!
 - *PIXE + Backscattering – self-consistent analysis*
 - **Accurate analysis!**
- The $^{28}\text{Si}(\alpha,\alpha)^{28}\text{Si}$ reaction
- Summary

First *critical* 1% accuracy RBS report, 2012

**analytical
chemistry**

dx.doi.org/10.1021/ac300904c

Article

pubs.acs.org/ac

Accurate Determination of Quantity of Material in Thin Films by Rutherford Backscattering Spectrometry

C. Jeynes,^{*,†} N. P. Barradas,[‡] and E. Szilágyi[§]

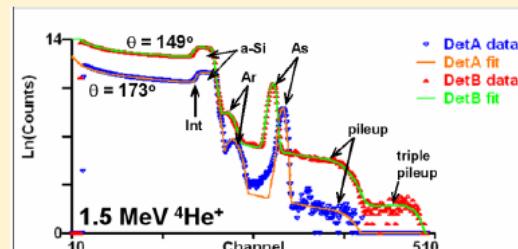
[†]University of Surrey Ion Beam Centre, Guildford, England

[‡]Instituto Superior Técnico/ITN, Universidade Técnica de Lisboa, Sacavém, Portugal

[§]Institute for Particle and Nuclear Physics, Wigner Research Centre for Physics, Budapest, Hungary

Supporting Information

ABSTRACT: Ion beam analysis (IBA) is a cluster of techniques including Rutherford and non-Rutherford backscattering spectrometry and particle-induced X-ray emission (PIXE). Recently, the ability to treat multiple IBA techniques (including PIXE) self-consistently has been demonstrated. The utility of IBA for accurately depth profiling thin films is critically reviewed. As an important example of IBA, three laboratories have independently measured a silicon sample implanted with a fluence of nominally 5×10^{15} As/cm² at an unprecedented absolute accuracy. Using 1.5 MeV ${}^4\text{He}^+$ Rutherford backscattering spectrometry (RBS), each lab has demonstrated a combined standard uncertainty around 1% (coverage factor $k = 1$) traceable to an Sb-implanted certified reference material through the silicon electronic stopping power. The uncertainty budget shows that this accuracy is dominated by the knowledge of the



1% absolute (traceable) accuracy on ion implant fluence of 5.10^{15} As/cm² with RBS (2 detectors) fully corrected for pulse pileup and pulse height defect.

C. Jeynes, N.P.Barradas, E. Szilágyi, *Analytical Chemistry*, 84(14) (2012) 6061-6069

Contents

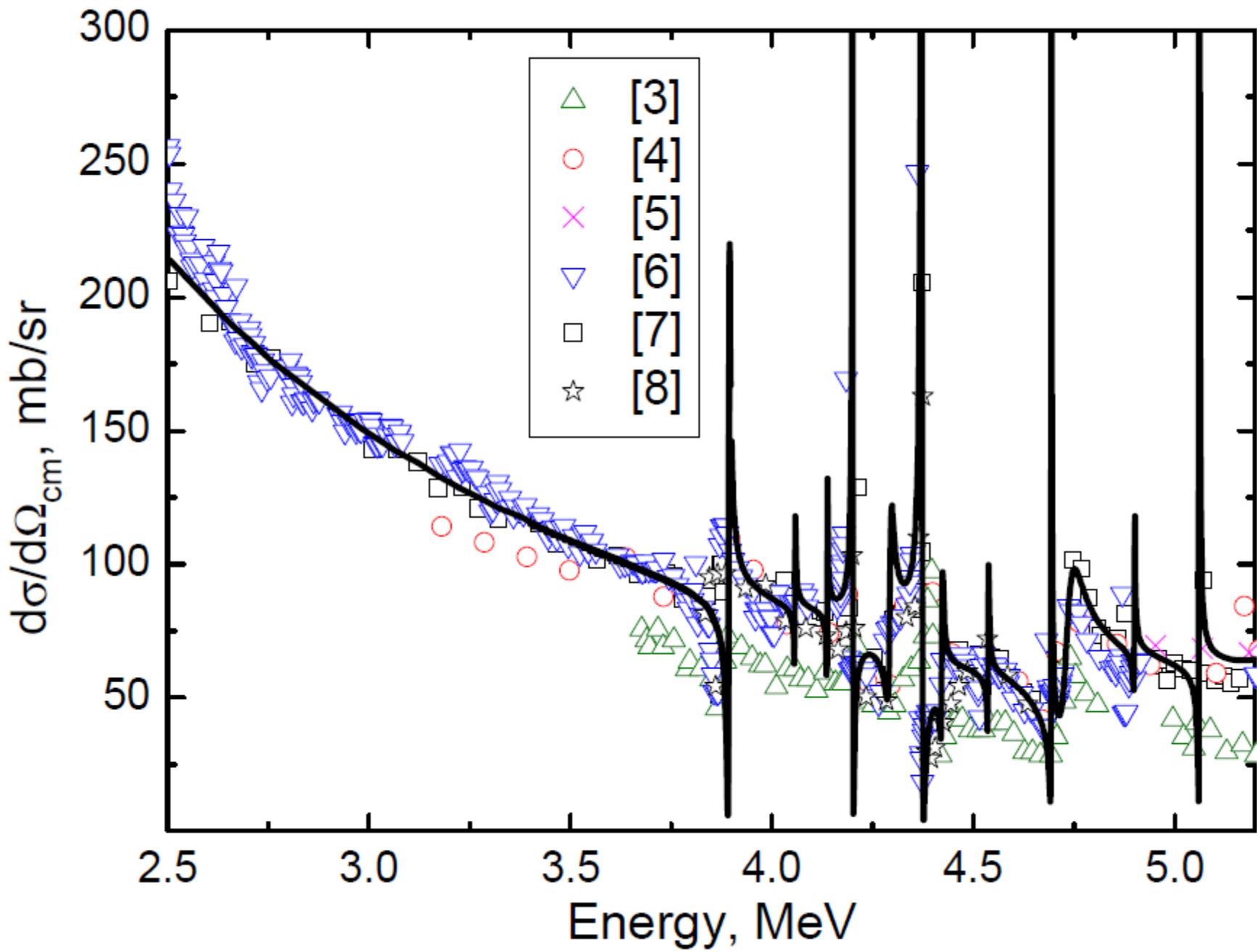
- Introduction – Materials Analysis
- The $^{28}\text{Si}(\alpha,\alpha)^{28}\text{Si}$ reaction
 - *Why?*
 - *Previous work*
 - *R-matrix modelling*
 - *Beam Energy*
 - *Benchmarking*
 - *Results*
- Summary

Why Silicon (α,α)?

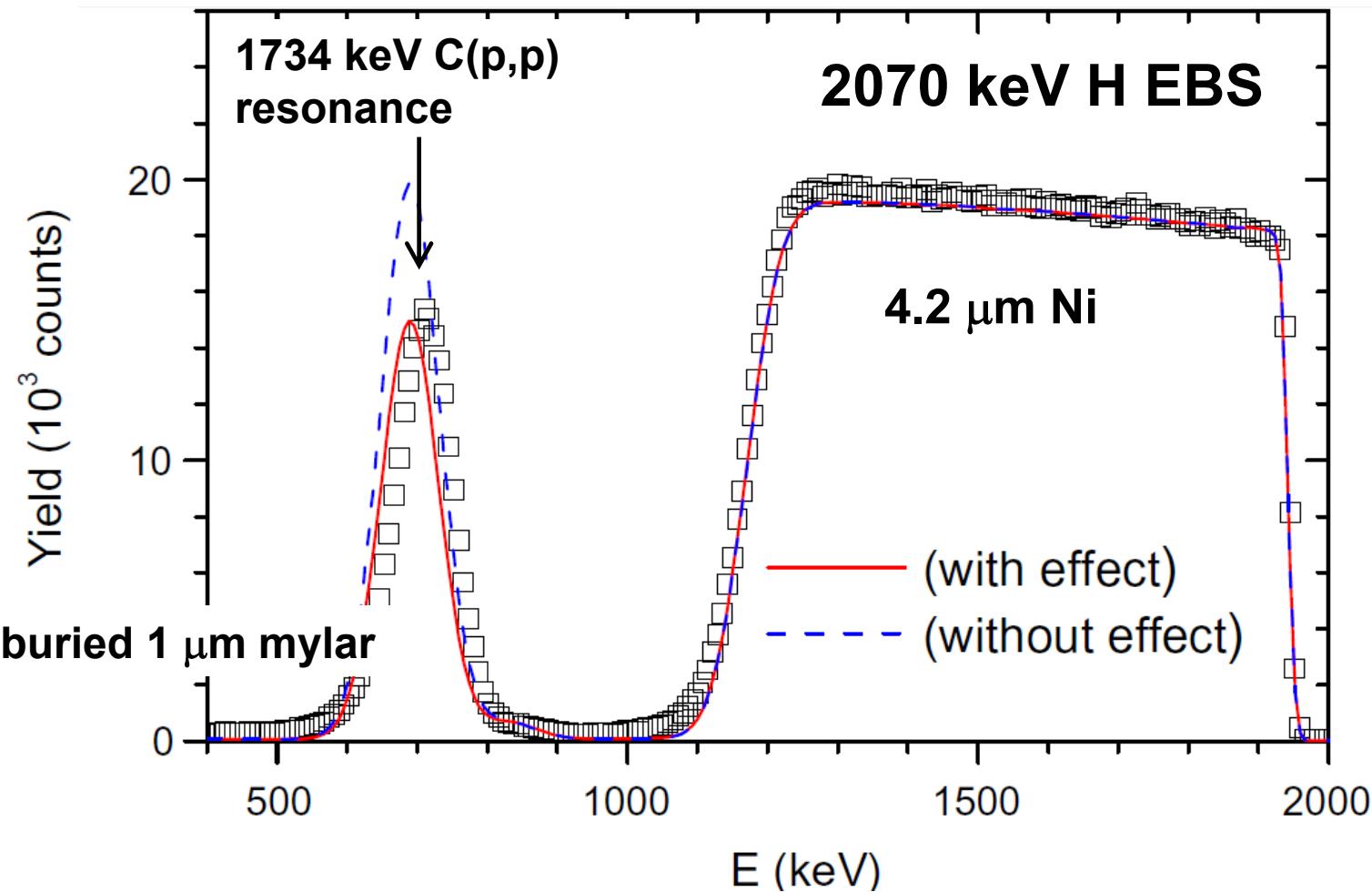
- Silicon
 - ***Important semiconductor material***
 - ***2nd most abundant element in the earth's crust***
- Si is the matrix for many samples of interest – without Si cross-sections we cannot use EBS!
 - ***For example, the strong $^{12}\text{C}(\alpha,\alpha)^{12}\text{C}$ resonance at 4262 keV***
 - ***For example, the strong $^{14}\text{N}(\alpha,\alpha)^{14}\text{N}$ resonance at 4475 keV***
 - ***For example, thick samples need high energy***
- Si is important in the stellar nucleosynthesis α process
 - ***^{28}Si is 8th and ^{32}S is 10th most abundant element in Universe***
 - ***Elastic scattering cross-sections central to the nuclear model***
 - ***Astrophysics interest***

Previous Work: $^{28}\text{Si}(\alpha, \alpha)^{28}\text{Si}$ measurements

- K.-M. Källman, *Zeitschrift für Physik A*, 356, 287 (1996); 3.6 – 5.8 MeV, 19 angles 173°-82°, thick film target; R-matrix analysis (reported in Nuclear Data Sheets 2011)
- A. Coban, F.Z. Khiari, M.S. Abdelmonem, A. Aksoy, A.A. Naqvi, *Nuclear Physics A* 678, 3 (2000); 130° to 170° with 10° step; 3.1 – 7.7 MeV
- J.J. Lawrie, A.A. Cowley, D.M. Whittal, S.J. Mills, W.R. McMurray, *Zeitschrift für Physik A*, 325, 175 (1986); 168°, 126°, 89°, 70°; 4.9 - 11.7 MeV
- M.K. Leung, Ph.D. dissertation, Univ. of Kentucky (1972); 165°, 2.5 - 6 MeV
- H.-S. Cheng, H. Shen, F. Yang, J.-Y. Tang, *Nuclear Instruments and Methods in Physics Research B* 85, 47 (1994); 170°, 2 – 9 MeV
- R. Somatri, J.F. Chailan, A.Chevarier, N.Chevarier et al., *Nucl. Instrum. Methods in Physics Research B* 113, 284 (1996); 172°, 3.8 – 4.6 MeV



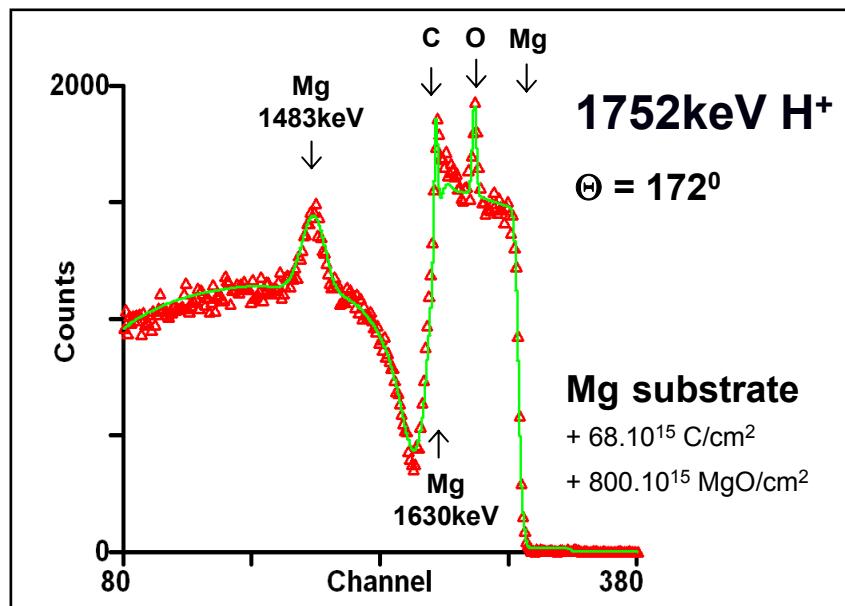
Previous Work: spectral simulation code



N.P.Barradas & C.Jeynes, Nucl. Instrum. Methods B, 266 (2008) 1875-1879

DataFurnace (NDFv.9) code to calculate **sharp resonances** correctly

Previous Work: spectral simulation code

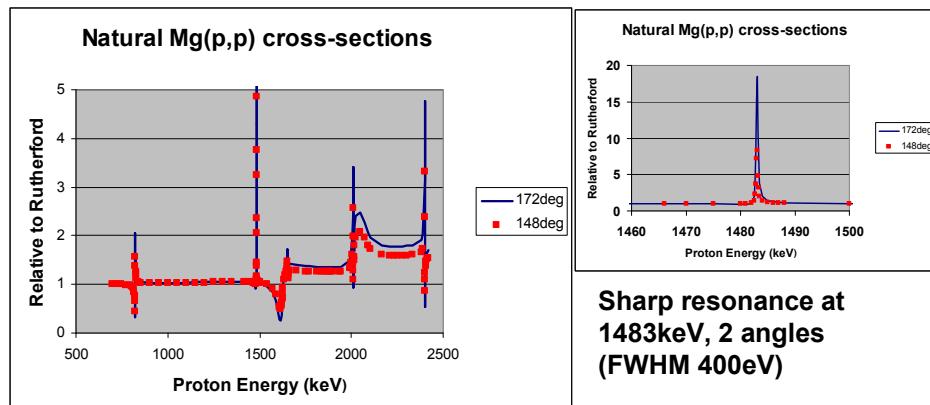


Benchmark experiment for evaluated Mg cross-sections

Gurbich & Jeynes, Nucl.Instrum.Methods B265 (2007) 447-452

EBS

- Kinematics the same as for RBS
 - Scattering cross-sections not Coulomb
 - Can be fitted by solving Schrödinger's equation
 - See **SigmaCalc** at www-nds.iaea.org/ibandl
- Gurbich, NIM B268 (2010) 1703**
- *Greatly enhanced* cross-sections often available for light elements
 - Cross-sections vary strongly with scattering angle



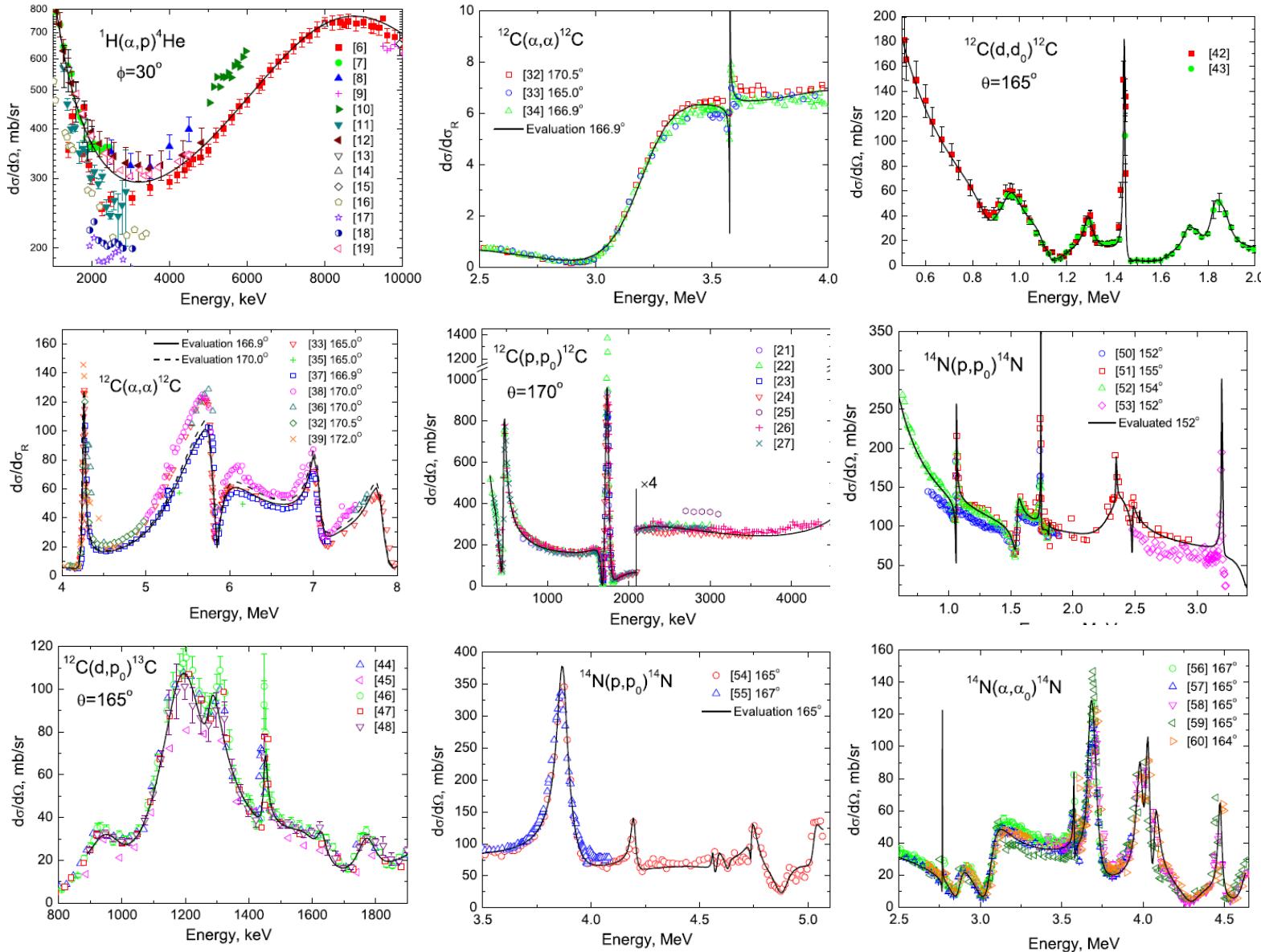
SigmaCalc scattering cross-sections for natural Mg (the isotopes behave differently) at two different scattering angles

For sharp resonances one must correctly calculate energy straggling in depth (this effect can be LARGE)

Barradas et al, NIM B247 (2006) 381

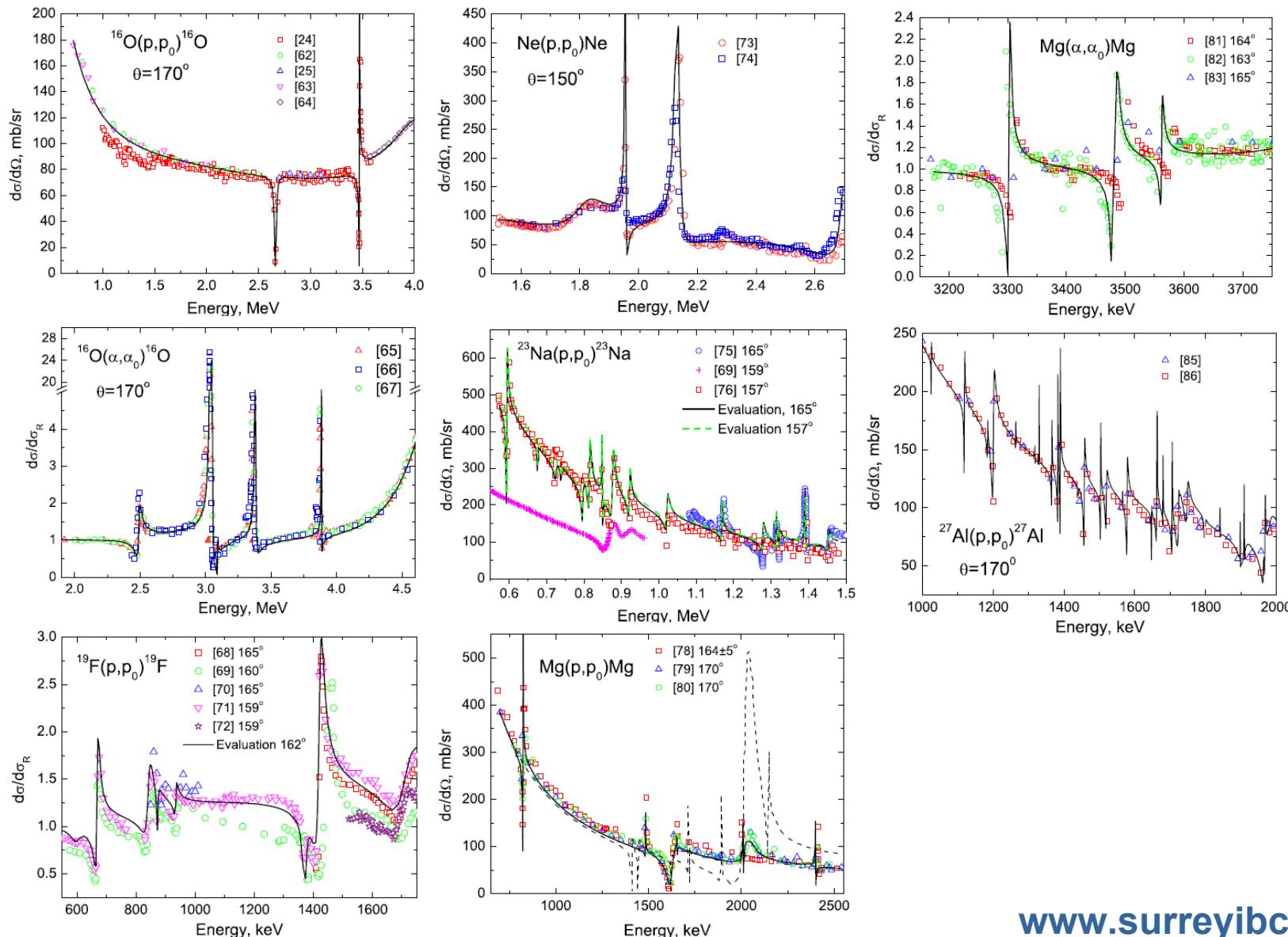
Previous Work: evaluations

A.F.Gurbich, Nucl.Instrum.Methods B, 268 (2010) 1703-1710



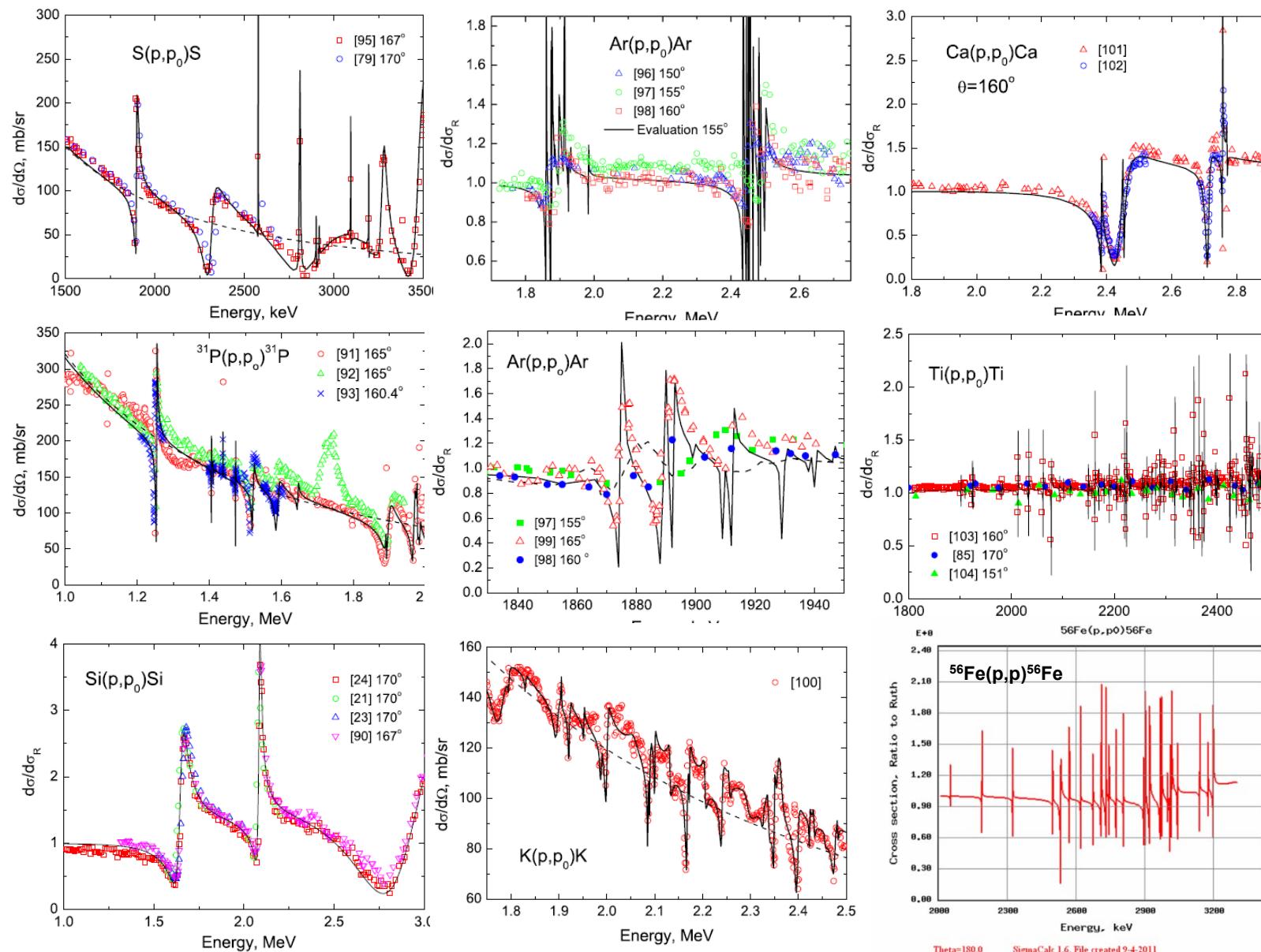
Previous Work: evaluations

A.F.Gurbich, Nucl.Instrum.Methods B, 268 (2010) 1703-1710

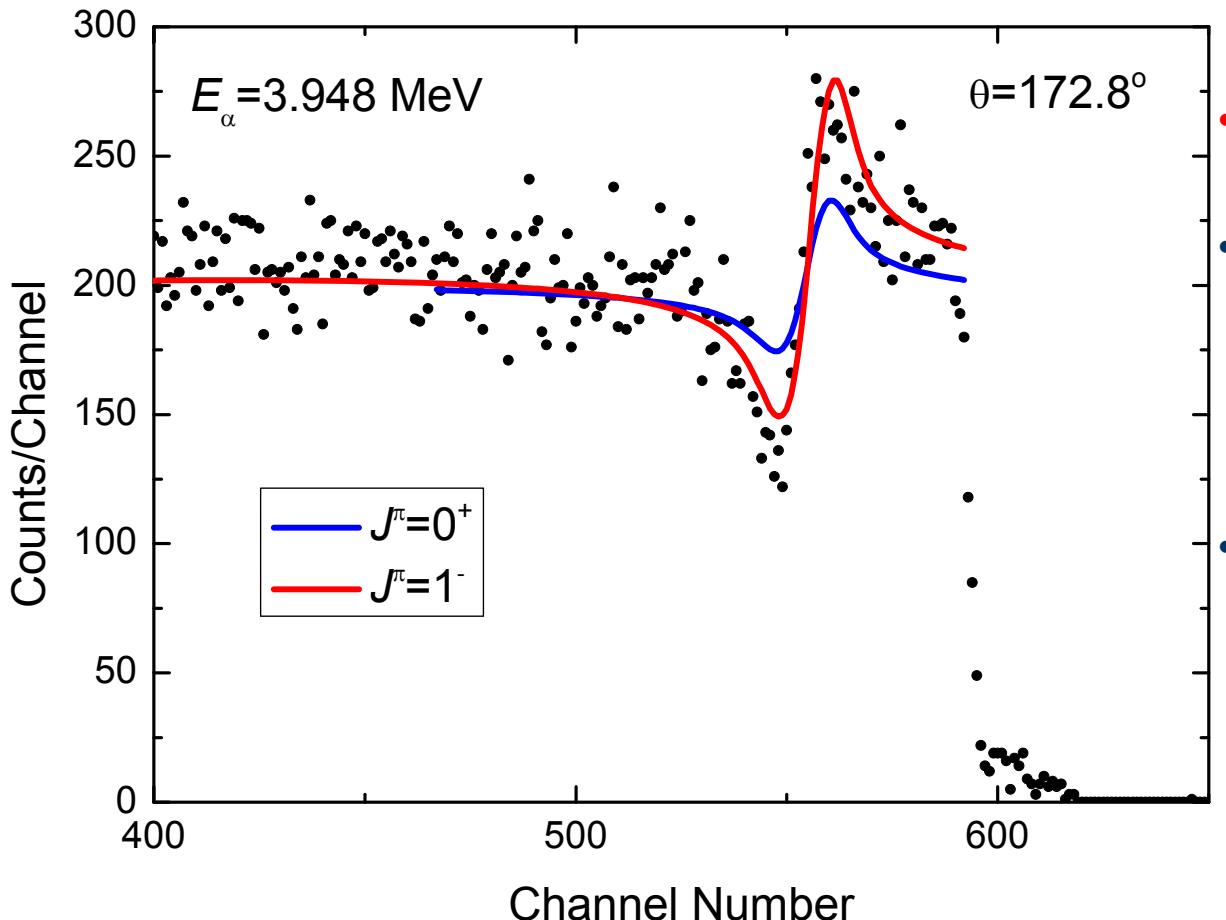


Previous Work: evaluations

A.F.Gurbich, Nucl.Instrum.Methods B, 268 (2010) 1703-1710



R-matrix modelling

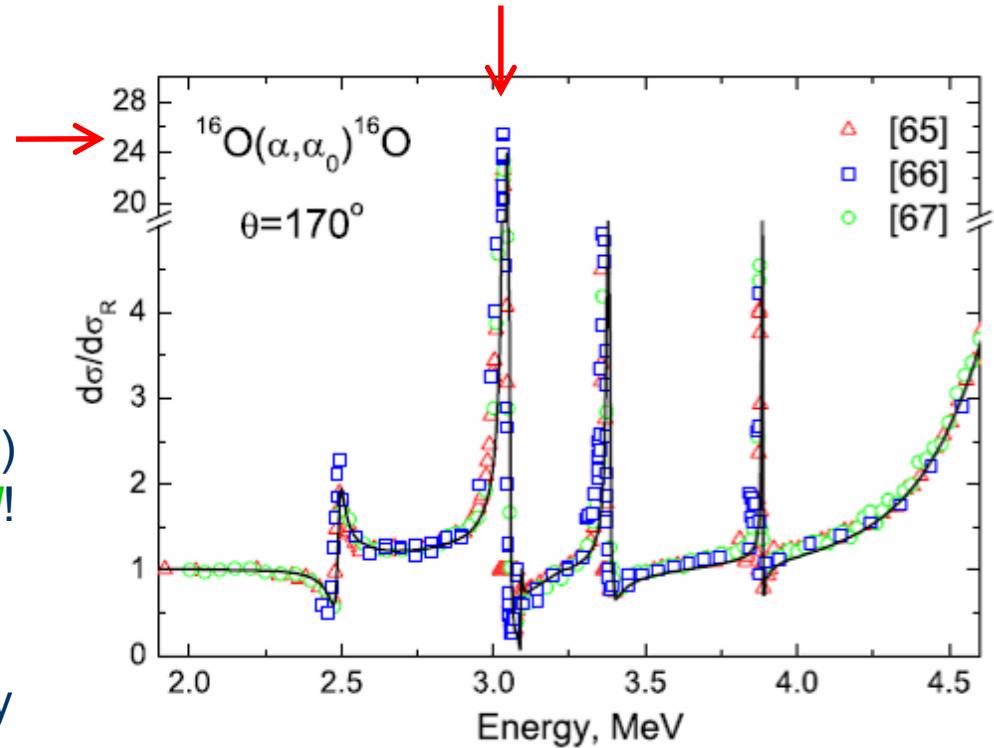


See: A.F.Gurbich, Evaluation of non-Rutherford proton elastic scattering cross section for nitrogen, *Nucl.Instrum.Methods B*, 266 (2008) 1193–1197

Finding the beam energy:

using EBS resonances as calibration points

- Schrödinger's equation solved for all open channels in nuclear scattering problem (see Gurbich 2010)
- Free parameters determined using nuclear data (including measured scattering cross-sections)
- For critical applications (where Uncertainty Budgets are constructed) RBS and EBS must be *distinguished!*
- Dramatically enhanced EBS sensitivities at resonances.
- Resonances can be used analytically where evaluated data exist.
- This resonance is at **3038±1 keV** (see current SigmaCalc)



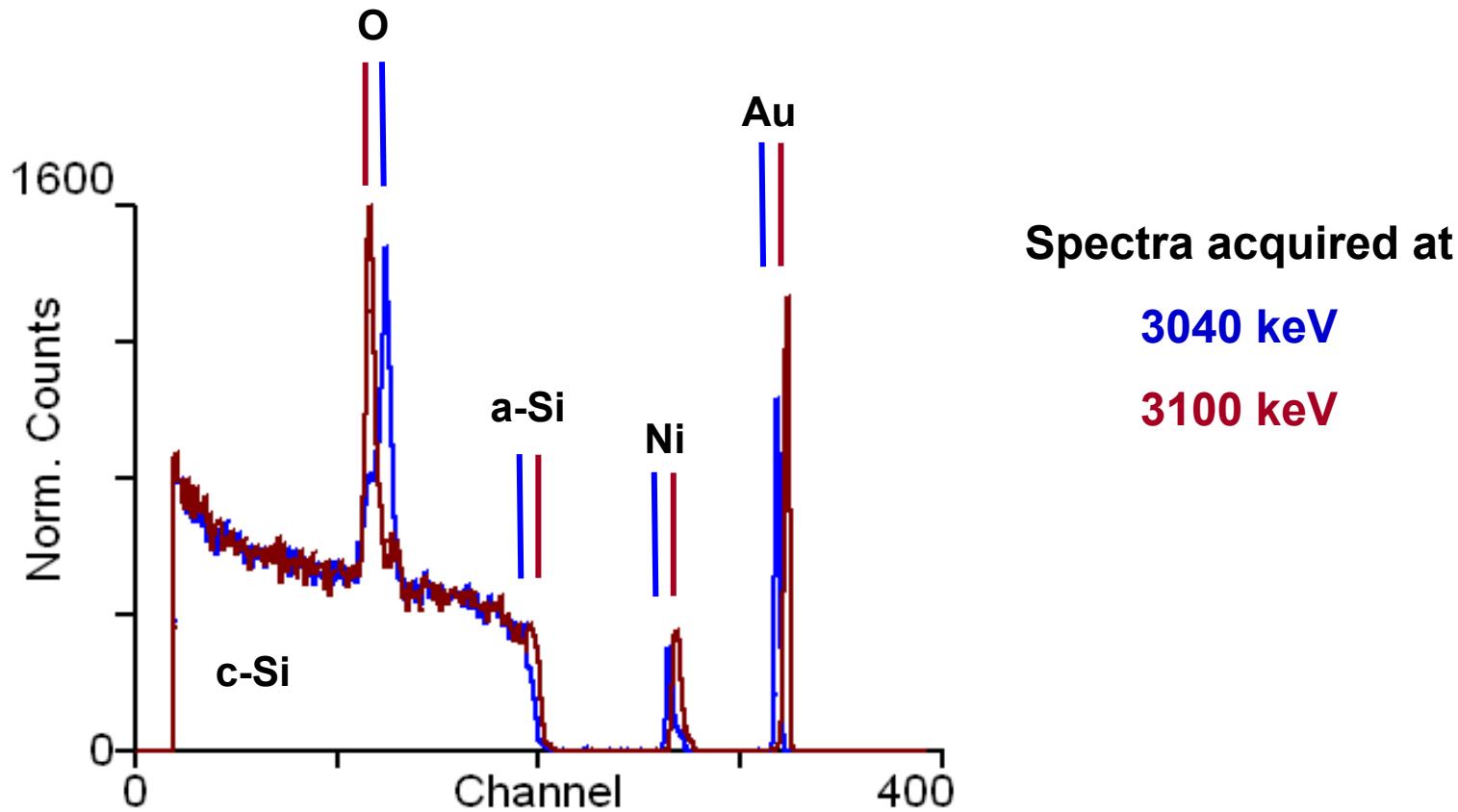
IBANDL (IBA Nuclear Data Library) :- www-nds.iaea.org/ibandl

SigmaCalc (evaluated cross-section on-line calculator) :- www-nds.iaea.org/sigmacalc

A.F.Gurbich, "The interaction of charged particles with nuclei", Chapter 3 in **2010 Handbook of Modern IBA** (Y.Q.Wang & M.Nastasi, eds, 2nd Ed., Pittsburgh: MRS)

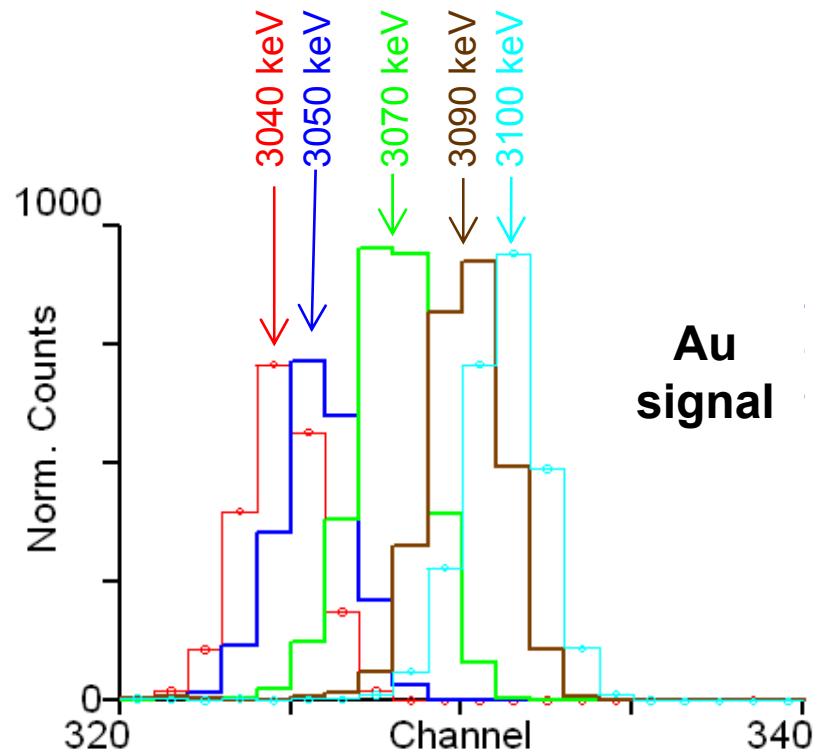
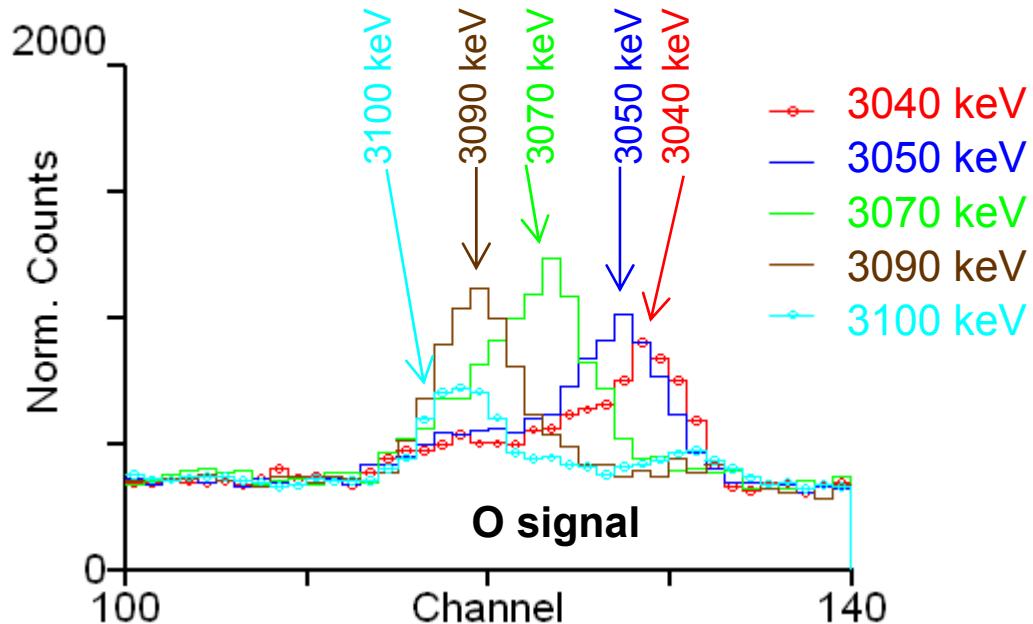
Finding the beam energy

- Use Si\SiO₂\Ni\Au sample
- Channel to reduce background on O signal (not essential)
- Gain (hence PHD) determined *directly* by sample



Finding the beam energy

- Use Si\SiO₂\Ni\Au sample
- Channel to reduce background on O signal (not essential)
- Gain (hence PHD) determined *directly* by sample
- Multiple spectra at multiple energies
- Spectral shape determines energy (*fitting* in NDF)
- ¹⁶O(α, α)¹⁶O resonance at **3038 ± 1 keV**



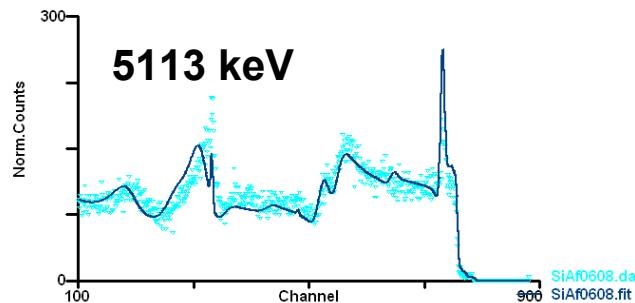
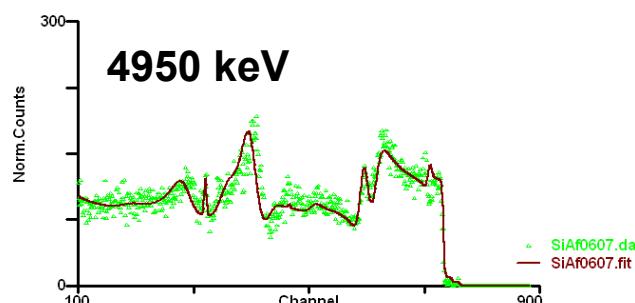
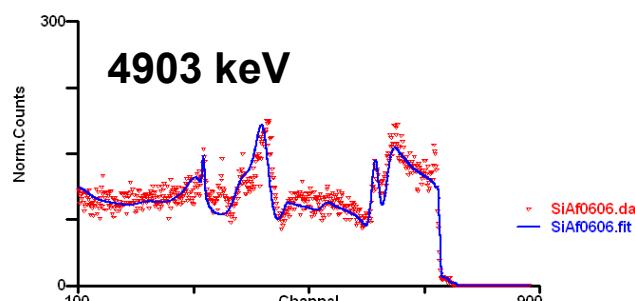
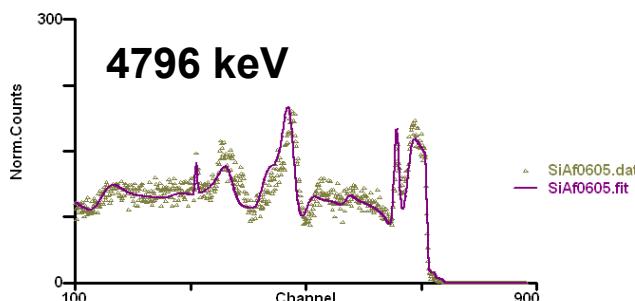
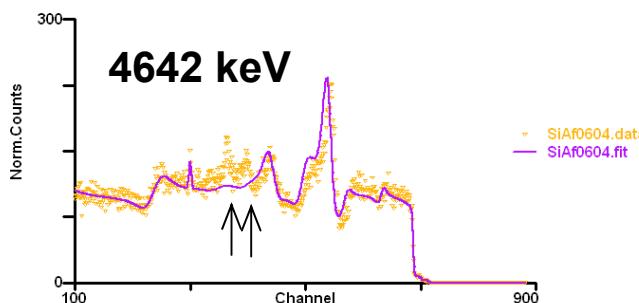
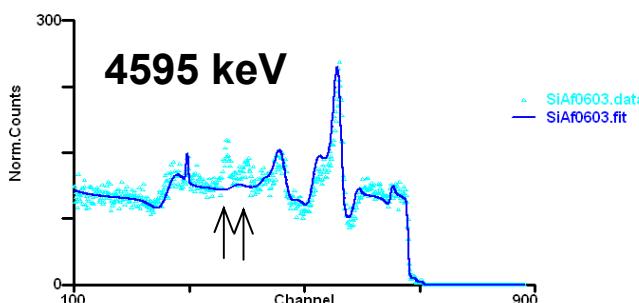
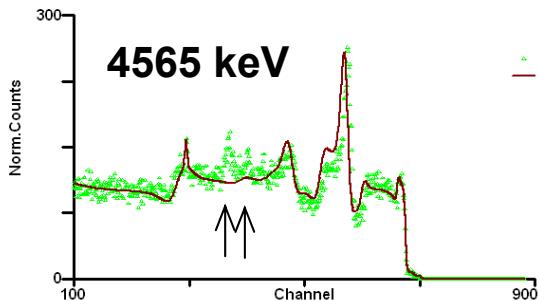
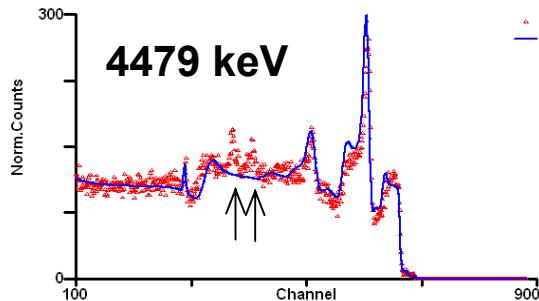
Finding the beam energy

- $\text{DetA}/\text{DetB} = 1 + 0.05\%$. This is a **fitting bias**.
- DetA/DetB uncertainty is **0.03%**. This is a **fitting uncertainty**.
- Calibration factor uncertainty is **0.07%**. This can be interpreted as a **set-voltage uncertainty** of **1 kV** (or an energy uncertainty of 2 keV)

Nominal Voltage kV	Fitted			Ratio Det A / Det B	Calibration factor
	Det A (keV)	Det B (keV)	Average (keV)		
1495	3019.90	3020.00	3019.95	0.999967	1.0033
1500	3030.80	3030.10	3030.45	1.000231	1.0035
1505	3040.10	3039.60	3039.85	1.000164	1.0033
1510	3055.40	3053.40	3054.40	1.000655	1.0048
1515	3065.30	3063.60	3064.45	1.000555	1.0048
1520	3076.30	3073.50	3074.90	1.000911	1.0049
1525	3085.80	3083.30	3084.55	1.000811	1.0048
1530	3095.10	3093.20	3094.15	1.000614	1.0046
1535	3102.80	3102.20	3102.50	1.000193	1.0041
NB: fixed gain & PHD!		Average		1.000456	1.0042
		St deviation		0.031%	0.065%

Contents

- Introduction – Materials Analysis
- The $^{28}\text{Si}(\alpha,\alpha)^{28}\text{Si}$ reaction
 - *Why?*
 - *Previous work*
 - *R-matrix modelling*
 - *Beam Energy*
 - *Benchmarking*
 - *Results*
- Summary



Set of data :-

2 detectors

$\sim 150^\circ$ & 170°

78 energies

3717 – 6167 keV

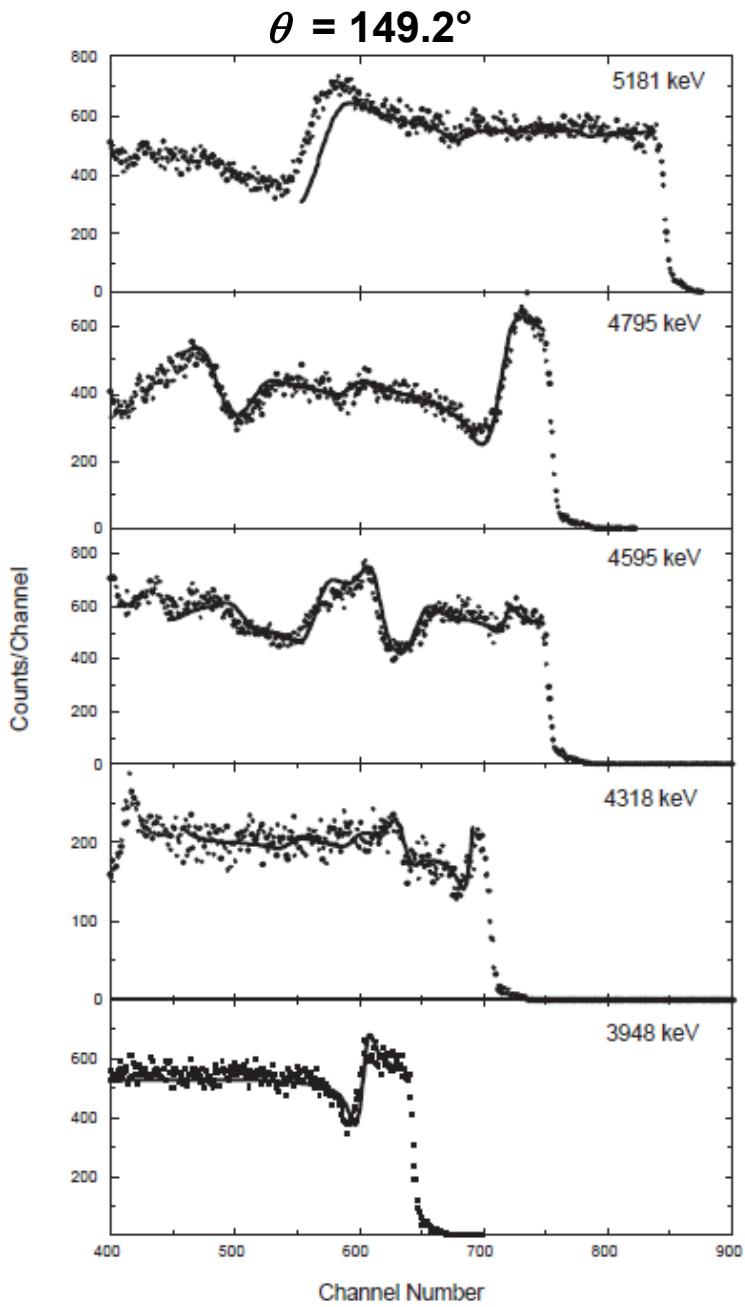
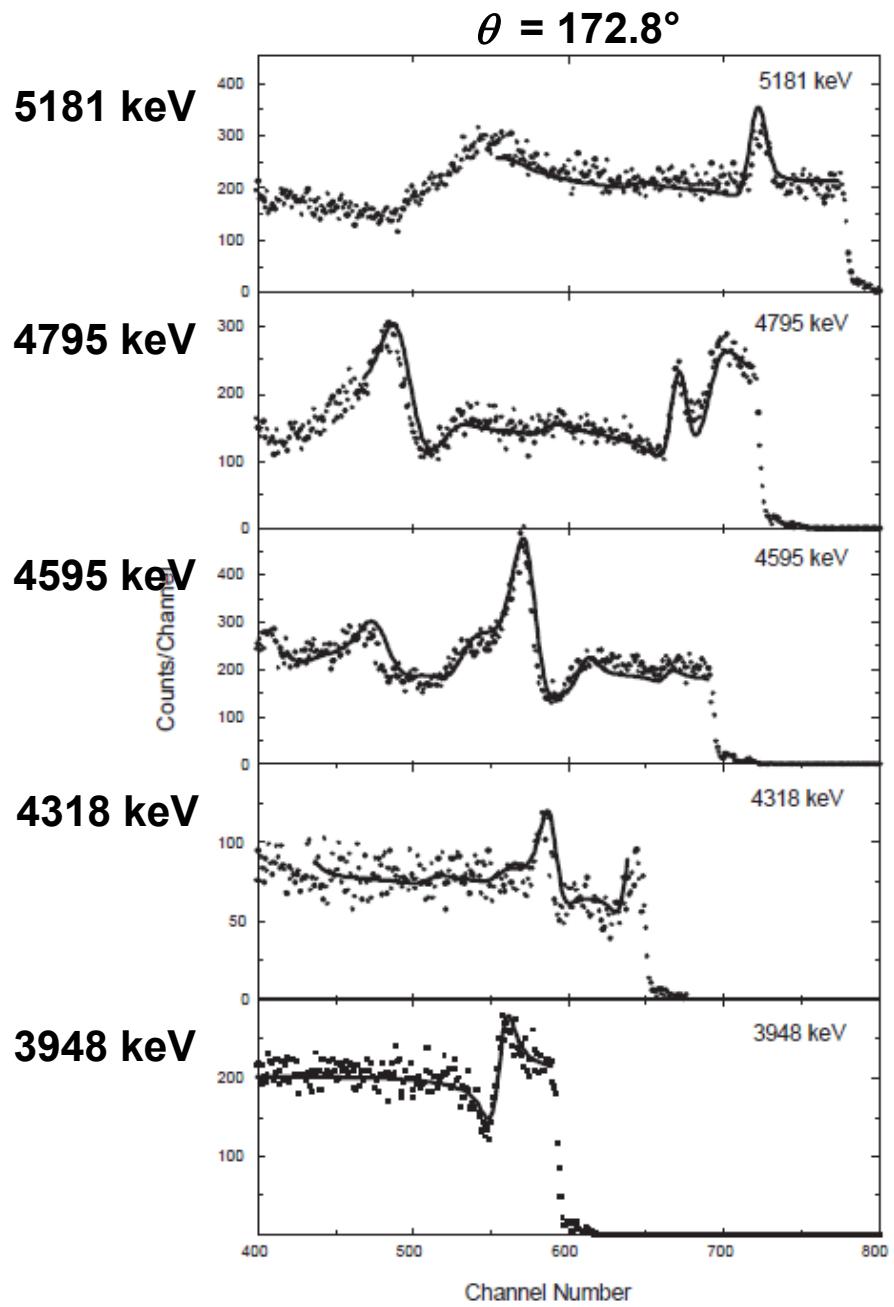
Energy calibration:

3038 keV $^{16}\text{O}(\alpha, \alpha)$

4262 keV $^{12}\text{C}(\alpha, \alpha)$

± 4 keV systematic

± 2 keV random



Results

E _x (keV)			J _π			Γ (keV)		
NPA 1990	NDS 2011	Surrey	NPA 1990	NDS 2011	Surrey	NPA 1990	NDS 2011	Surrey
10332	10369	10340	1-	(0+)	1-	6.1	5.8	3.6
10457	10500	10500	0+	(0+)	0+	1.7	1.7	1.7
10550	10570	10570	0	(0+)	0+	8	1.2	1.2
10701	10658	10623	1-	(1-)	3-	21	2.3	1.3
10769	10745	10718	2-	(0+)	0+	5.1	8.9	8.9
---	10816	10781		(3-, 5-)	3-		4.7	3.3
10826	10868	10824	1-	(2+)	0+	22	7.7	4.7
10916	10956	10921	1-	(0+)	0+	1.6	2.9	1.9
---	11107	11054		(2+)	0+		67.4	0.6
11140	11130	11166	1+	(0+)	5-	2.6	1.8	6.7
---	11254	11236		(3-)	2+		1.1	2.1
---	11410	11383		(3-)	5-		1.9	0.6

- NPA1990: P.M.Endt, *Nuclear Physics A*, 521 (1990) 1-830
- NDS2011: C.Ouellet & B.Singh, *Nuclear Data Sheets* 112 (2011) 2199-2355. These values in NDS2011 are based on K.-M.Källman, *Z. Phys. A*, 356 (1996) 287-291

Summary

- Accurate EBS cross-sections are:
 - **essential for IBA (PIXE + backscattering)**
 - **valuable also for astrophysics!**
- Evaluated cross-sections:
 - ***Thin targets are best for making measurements***
 - ***Thick targets are best for benchmarking***
 - ***R-matrix fitting, Saxon-Woods absorption (not hard sphere)***
- Set of EBS spectra:
 - ***Very accurate detector calibration valid for whole set***
 - ***Very accurate 2 MV HVEE Tandetron calibration (4 keV systematic from known EBS resonances; 2 keV random from setting errors)***
 - ***Correlation of all reactions reduces uncertainty***
 - ***Ex, J π and Γ values from spectral data***
 - ***Values contradict NDS***

Thanks for listening!



Ion Beam Analysis : amazingly powerful!