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Pitfalls in Depth Profiling II

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Pitfalls in Depth Profiling **II**

Joint ICTP/IAEA Workshop on Advanced Simulation and Modelling for Ion Beam Analysis

23 - 27 February 2009, Miramare - Trieste, Italy

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Pitfalls In Ion Beam Analysis

Chapter in the forthcoming updated IBA Handbook

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J. A. Davies, W. N. Lennard and I.V. Mitchell;
responsible for the Pitfalls chapter in the 1994 IBA Handbook

Context

- Elemental depth profiling : what is our competitive edge compared with other techniques (e.g. SIMS)?

IBA	SIMS
Quantitative	Small footprint
Good at interfaces	High sensitivity

- IBA spectra can be treated with a numerical confidence of **0.2%***
- Best available absolute experimental accuracy is **0.6%***
- We should be aiming for absolute accuracy of **1%** or better

* *Barradas et al: NIMB262 (2007) 281-303, summary at NIMB266 (2008) 1338-1342*

2009 Handbook Pitfalls Chapter Contents

Note: here we will consider only spectral handling (not data collection) pitfalls

- Lost Beam and Events
- **Fixed Parameter Calibration (gain, geometry, resolution)**
- Algorithmic Issues (Matej)
- **Accurate IBA (uncertainty estimation)**
- Unwanted Beam-Target Interactions
- Other Effects
- Summary

We want to interpret the spectra correctly

How do we evaluate the uncertainties?

Which parameters do the spectra tell us?

Which parameters must we know precisely to interpret the spectra?

Chapter contents

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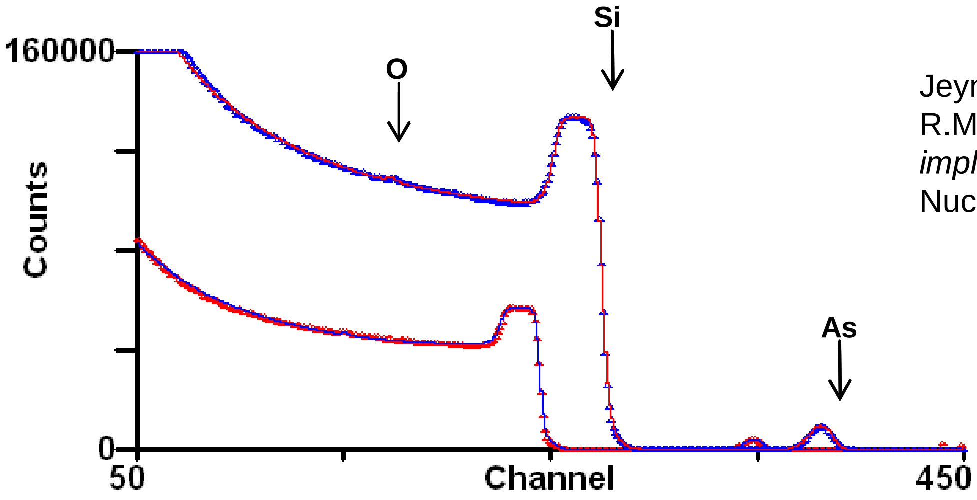
Notes:

Charge.solid-angle product is always uncertain – this is considered in "Ambiguity" talk

Electronic Gain



Jeynes C., Peng N., Barradas N.P., Gwilliam R.M. (2006), *Quality assurance in an implantation laboratory by high accuracy RBS*, Nucl. Instrum. Methods B249: 482-485

Why is gain Δ important?

$\mathbf{A_A} = Q\, N_A\, \sigma'_A\, (E, \theta)\ \ \Omega$ not for number of counts!

$\mathbf{Y_{0,A}} = Q\, f_A\ \ \sigma'_A\ \ \Omega\, \Delta\, / \,[\, \varepsilon_0 \,]\, _A{}^{AB}$ but to get Q * Ω

Electronic Gain

How precisely can it be obtained?

- Seah *et al*, 1988: <0.5% *An intercomparison of absolute measurements of the oxygen and tantalum thickness of tantalum pentoxide reference materials, BCR 261, by 6 laboratories,* Nucl. Instr. Methods **B30,** 140-151
- Munnik *et al,* 1996: 0.16% F. Munnik, A.J.M. Plompen, J. Räisänen, U. Wätjen*, Stopping powers of 200-3000 keV 4He and 550-1750 keV 1H ions in Vinyl,* Nucl. Instr. Methods **B119**, 445-151
- Bianconi *et al*, 2000: 0.2% reported in Barradas et al: Nucl. Instr. Methods **B262** (2007) 281-303
- Gurbich & Jeynes, 2007: <0.1% (PHD corrected) *Evaluation of non-Rutherford proton elastic scattering cross section for magnesium*, Nucl. Instr. Methods **B265** 447-452

Pulse Height Defect

- Detector non linearity (gain varies across energy range). Arises from:
  - Energy loss in detector dead layer / entrance window
  - Nuclear (non-ionising) energy loss (NIL) of projectile in the detector
  - Radiation damage in the detector (recombination sites)
- NIL can be accounted for using Lennards' correction

  (W.N. Lennard, S. Y. Tong, G. R. Massoumi, L. Wong, Nucl. Instr. & Methods ***B45*** *(1990) 281-284)*

Pulse Height Defect

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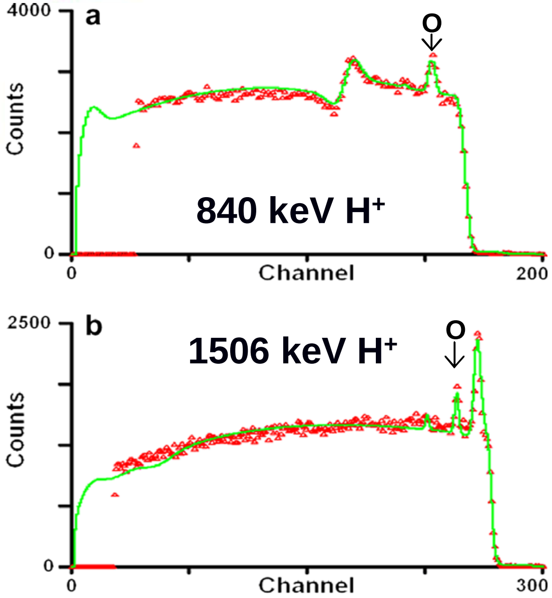
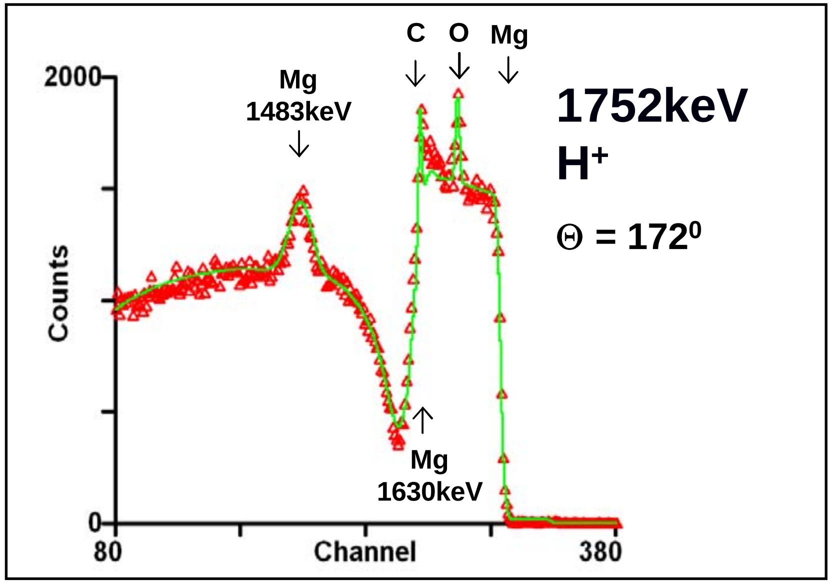
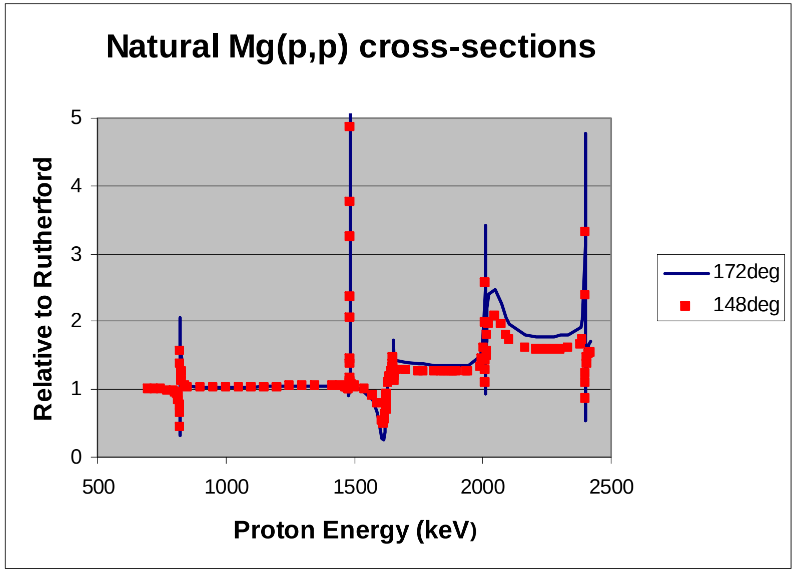


Bulk Mg target



Gurbich & Jeynes, NIM **B265** 447-452



(Left) Spectra of bulk magnesium with 68.10^{15} C/cm^2 and 800.10^{15} MgO/cm^2 on the surface

(Above) SigmaCalc scattering cross-sections for natural Mg (the isotopes behave differently) at two different scattering angles with sharp resonance at 1483keV (FWHM 400eV)

- Gain uncertainty is <0.1% if PHD is accounted for
- Gain changes by 5% over dataset without PHD
- Important if spectra from different ions or energies are to be compared

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Electronic Gain

$$E = \Delta C + o$$

energy E of channel C depends on gain Δ and offset o

I have never seen non-linearity, if PHD correction is used

- Do we care about the offset?
- No, but we need to determine ***both*** o & Δ (correlated variables)
  for Gurbich & Jeynes 2007, o was determined at <1keV for both detectors independently
- Isn’t this an experimental problem?
- No, it’s a ***data analysis*** problem

Electronic Gain

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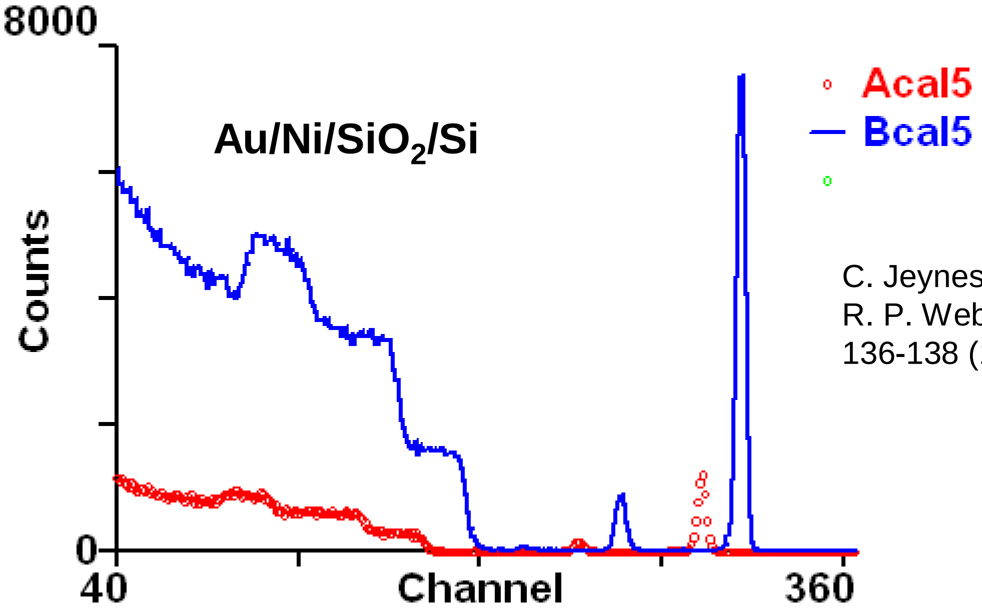

C. Jeynes, N. P. Barradas, M. J. Blewett, R. P. Webb, Nucl. Instr. and Meth. B 136-138 (1998) 1229

- Peaks can be fitted at very high precision
- Edges can be fitted at high precision
- PROVIDED the ***detector resolution*** is known
- Multi-elemental sample is GOOD (doesn't matter if it is dirty)
- NB: gain(beam energy)
- Correction for energy loss in metal layers is easy

C. Jeynes, A.C.Kimber, *High accuracy data from RBS*, J.Phys.D, **18** (1985) L93-L97

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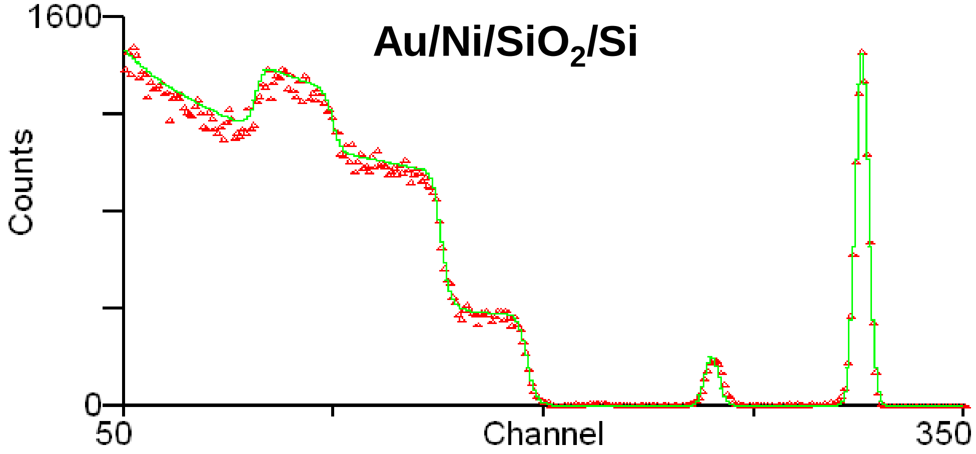
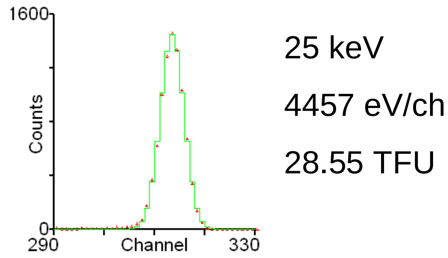
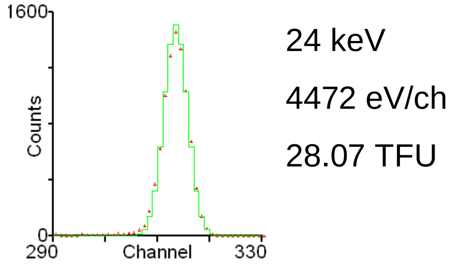
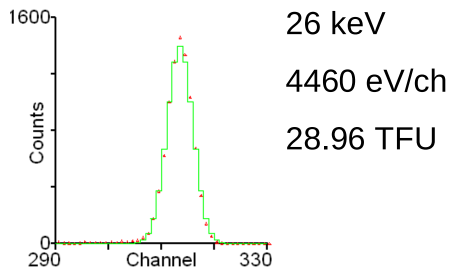
Detector Resolution



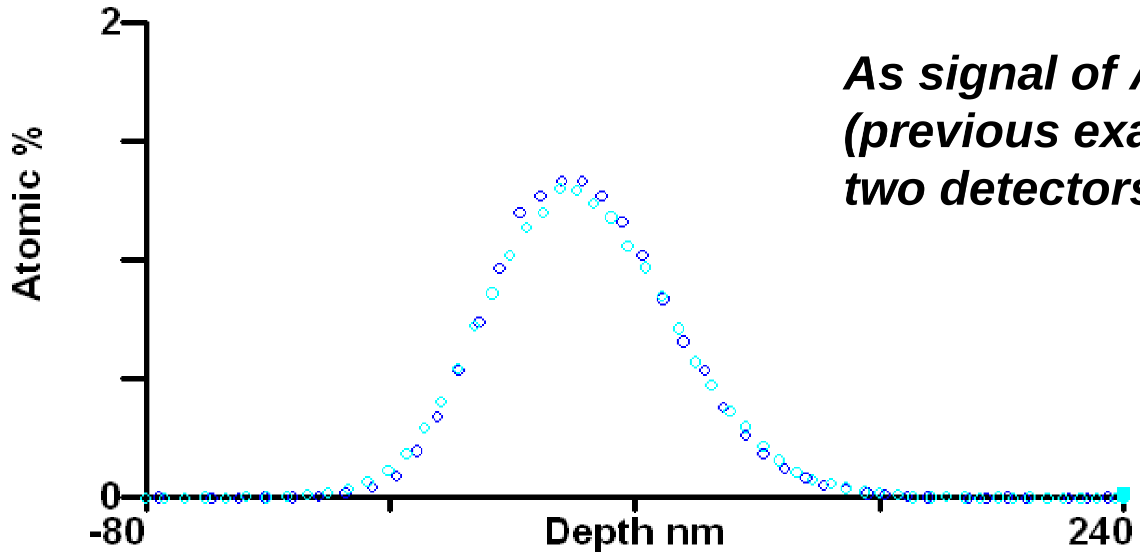






- 4% resolution change → 1.5% thickness change
- 4% resolution change → 0.25% gain uncertainty
- (need to control contributions to uncertainty at ¼%)

Electronic Gain



As signal of As implanted Si (previous example) two detectors

- Is it right?
- Why are the two signals different heights?
- ***Check***!

Chapter contents

Uncertainty

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- "Error" implies that you (or someone) has made a mistake
- "Uncertainty" expresses our ignorance of reality

Only God knows for sure!

- "Type A" uncertainty: obtained as a *variance* from ensemble of data
- "Type B" uncertainty: from a qualitative discussion

"GUM:1995" BIPM / IEC / IFCC / ISO / IUPAC / IUPAP / OIML

"***Guide to the expression of uncertainty in measurement*** ".

Identical to EN 13005:1999.

See also the valuable websites www.gum.dk, www.npl.co.uk/scientific_software/research/uncertainties.

Sjöland KA, Munnik F, Wätjen U, *Uncertainty budget for ion beam analysis*, Nucl. Instrum. Methods B161 (2000) 275-280

Uncertainty
Type A & Type B

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Think of measuring a length with a ruler

Type A: multiple measurements (perhaps by different people)

Type B: consideration of the spacing of the marks on the ruler and how well they could possibly be read (precision), checking whether the ruler is marked true (!), etc

Type A is good, but never sufficient!

We should remember always the famous case of the Astronomer Royal, Nicholas Maskeleyne, [in post 1765-1811] who dismissed his assistant Kinnebrook for persistently recording the passage of stars ***more than half a second later*** *than he, his superior. Maskeleyne did not realize that an equally watchful observer may register systematically different times by the method employed by him; it was only Bessel's realization of this possibility which 20 years later resolved the discrepancy and belatedly justified Kinnebrook.*

Michael Polanyi: *Personal Knowledge*, 1958

Table 2: Uncertainty Budget

coverage factor k=1

(Reproduced from Jeynes et al 2006 [ref2])

	Type A or B	IBM detector	Cornell detector	Comment
Pileup correction		2.60%	0.80%	
Uncertainty of pileup correction	A	2%	2%	From shape fitting accuracy
Counting statistics, As signal	A	0.28%	0.47%	
Counting statistics, a-Si signal	A	0.08%	0.13%	
Scattering angle	B	0.28%	0.07%	0.2° and ~$1/\sin^4\theta/2$
Electronic gain	B	0.5%	0.5%	
Pileup correction	A	0.05%	0.02%	See separate section above
Relative uncertainty		0.64%	0.70%	
Relative uncertainty of average of two detectors		0.48%		average / √2
Beam energy	B	0.20%		These are the same for both detectors
Rutherford cross-section	B	0.16%		Screening correction
Combined standard uncertainty		0.54%		Relative accuracy
IBA code uncertainty	B	0.2%		From software intercomparison (Barradas *et al* 2007) For HI-RBS this value is 0.7%, for He-ERD this value is 0.4%
Si stopping power	B	0.6%		From software intercomparison (Barradas *et al* 2007) since SRIM 2003 stopping powers were used
Total combined standard uncertainty		0.83%		Absolute accuracy

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C.Jeynes, N.Peng, N.P.Barradas, R.M.Gwilliam (2006), *Quality assurance in an implantation laboratory by high accuracy RBS*, NIM **B249**: 482-485

Revised in the light of the IAEA Software Intercomparison

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Final Observation

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The first attempt by the *leading labs*
at a Round Robin for RBS
showed charge measurement errors of 20%!

Davies, Lennard and Mitchell, Chapter 12, Black Handbook (1995)

It is *very easy* to make mistakes

We should beware!

Acknowledgements for 2009 IBA Handbook Pitfalls Chapter

- J. A. Davies, W. N. Lennard and I.V. Mitchell; responsible for the Pitfalls chapter in the 1994 IBA Handbook (the “Black Bible”), some of which is copied into this chapter
- Max Döbeli (Zurich) for the electronic noise and background loops section
- Alexander Gurbich for detailed comments