



The Abdus Salam
International Centre for Theoretical Physics



2015-2

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

23 - 27 February 2009

IBA IV IAEA Intercomparison

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The IAEA Intercomparison of IBA codes

*Joint ICTP/IAEA Workshop on Advanced Simulation and Modelling for
Ion Beam Analysis
23 - 27 February 2009, Miramare - Trieste, Italy*

Chris Jeynes

*University of Surrey Ion Beam Centre
Guildford, England*

Monday February 23rd 2009



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IAEA-sponsored intercomparison of IBA software codes



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Nuclear Instruments and Methods **B262** (2007) 281-303

summary at: Nuclear Instruments and Methods **B266** (2008) 1338-1342

This talk was presented at the IBA conference in Hyderabad, September 2007



<http://www.mfa.kfki.hu/sigmabase/ibasoft/>

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Context

- *Status of software for Ion Beam Analysis in Materials Development*, NAPC/PS/2002/F1.TM - 25886, (IAEA, Vienna 2003)
- E. Rauhala, N.P. Barradas, S. Fazinić, M. Mayer, E. Szilágyi, M. Thompson, *Status of ion beam data analysis and simulation software*, Nucl. Instr. Meth. B244 (2006) 436
- Barradas & Rauhala chapter on *IBA Software in new IBA Handbook* (this has been circulated on ION)
- *IAEA cross-section CRP*: A. Gurbich, I. Bogdanovic-Radovic, M. Chiari, C. Jeynes, M. Kokkoris, A.R. Ramos, M. Mayer, E. Rauhala, O. Schwerer, Shi Liqun and I. Vickridge, *Status of the problem of nuclear cross section data for IBA*, Nucl. Instrum. Methods Phys. Res., Sect. B, 266(2008)1198-1202
- PIXE & PIGE not considered here





Need for Intercomparison



- Ion Beam Analysis is an *accurate* and *traceable* technique
- IBA is *not trivial* to calculate:
 - The yield Ψ_e at detected energy E_3 for an element e is given by the triple integral:
(D.K.Brice, Thin Solid Films 19 1973, 121)
$$\Psi_e(E, E_3) = A \frac{\partial}{\partial E_3} \int_0^{\infty} dx' \int_0^t N_e dx \int_{E'}^E dE_1 P_{in} P_{out} \sigma(E_1)/S(E_1)$$
 - Even in the *single scattering* approx. the calculation is *intricate*
 - Many physical effects to take care of
- *New generation* single scattering codes
- *Monte Carlo* code available for comparison
- *IAEA* persuaded of need for support (cf IAEA support of IBANDL, SigmaCalc)



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Depth profiling codes



- *First Generation Single Scattering Codes*
 - Ziegler (1976)
 - GISA (Rauhala, 1984)
 - RUMP (Thompson, 1985)
 - RBX (Kótai, 1994)
- *Straggling Code*
 - DEPTH (Szilágyi, 1995)
- *New Generation Single Scattering Codes*
 - DataFurnace (“NDF” Barradas, Jeynes & Webb 1997)
 - SIMNRA (Mayer, 1997)
- *Monte Carlo Code*
 - MCERD (Arstila, 2000)





Overview of Intercomparison

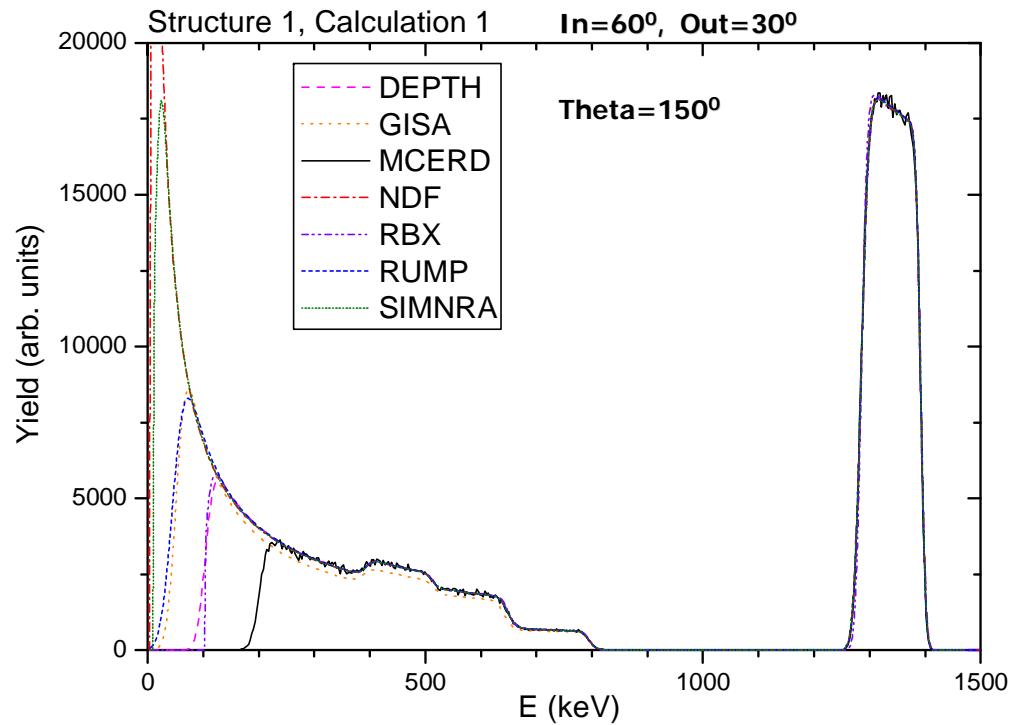
1. Comparative simulations
 1. Baseline RBS (sanity check)
 - a) Screening
 - b) Pileup
 - c) Double scattering
 2. Channelling
 3. EBS with sharp resonances O(a,a)O: (3.04 MeV ${}^4\text{He}$)
 4. ERD (1.5 MeV He)
 5. HI-RBS (3.5 MeV Li)
 6. HI-ERD (50 MeV I)
 7. NRA (1 MeV ${}^3\text{He}$)
 8. NRA (1 MeV D)
2. Detailed analysis of real spectra (RBS)
 1. a-Si spectrum (sanity check)
 2. IRMM certified Sb implant in Si
 3. HfO/Si sample
 4. Co-Re multilayer sample (roughness)



Baseline Calculation

Simulation of 50nm Au/200nm SiO₂/Si

(1.5MeV ⁴He⁺, Bohr straggling, 16keV detector resolution, single pure Rutherford scattering, no pileup, SRIM 2003)



All codes:

0.3% agreement: yield & height of various features

SIMNRA, DataFurnace & RUMP:

0.1% yield & height agreement
Surface & interface positions agree at 100eV

SIMNRA, DataFurnace:

Edge widths agree at 500eV



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Simulation of 50nm Au/200nm SiO₂/Si (1.5MeV ⁴He⁺, Bohr straggling, 16keV detector resolution, single Rutherford scattering with screening, no pileup, SRIM 2003)



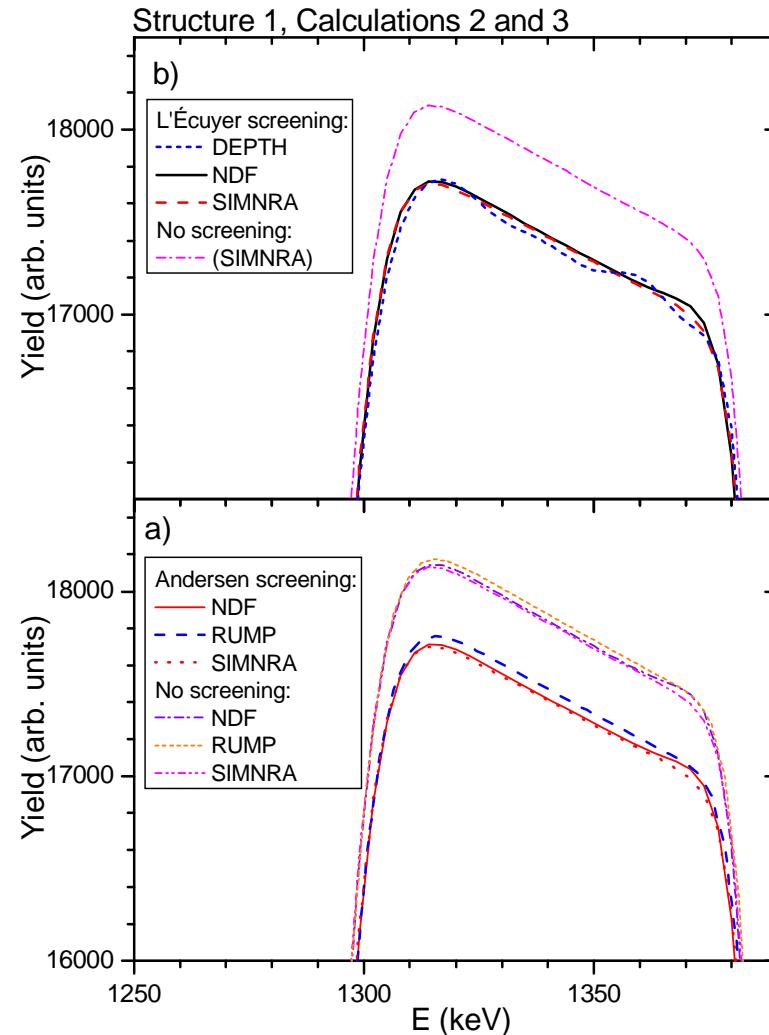
Same as previous, but with L'Ecuyer and Andersen screening

Gold signal

SIMNRA & DataFurnace
indistinguishable, RUMP very close



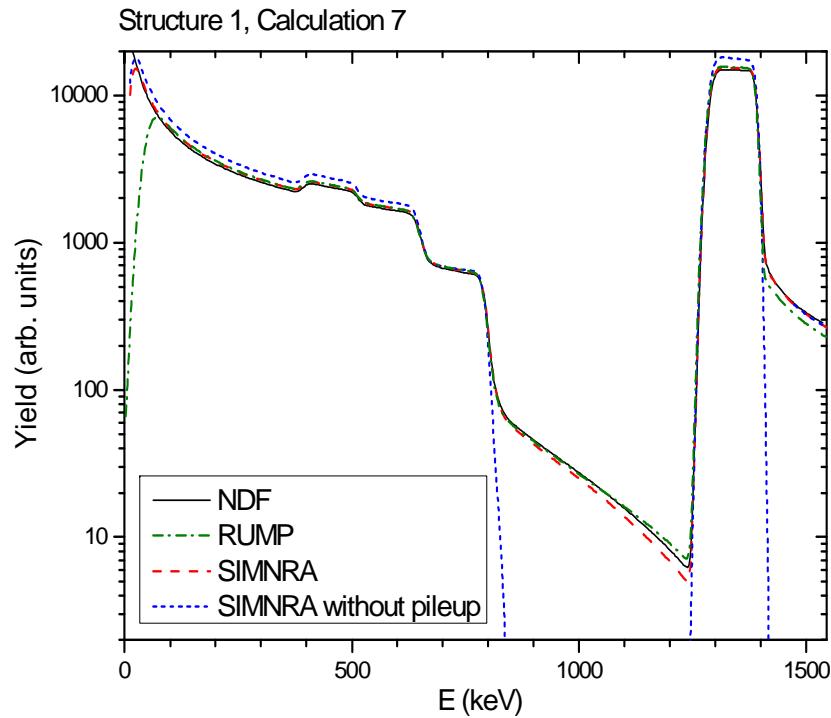
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Simulation of 50nm Au/200nm SiO₂/Si (1.5MeV ⁴He⁺, Bohr straggling, 16keV detector resolution, single pure Rutherford scattering, pileup no PUR, SRIM 2003)



Same as previous but with pileup and no pileup rejection

SIMNRA & DataFurnace almost indistinguishable: difference due to slight variation in pileup treatment
RUMP very close

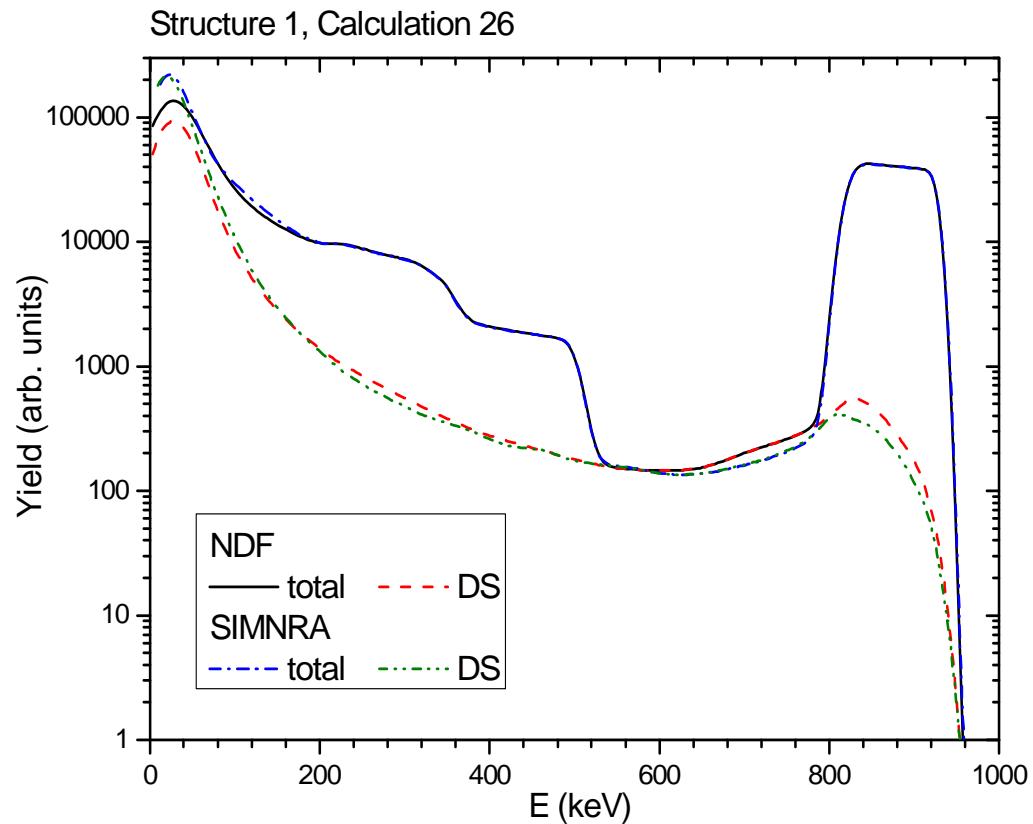


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Simulation of 50nm Au/200nm SiO₂/Si
(1MeV ⁴He⁺, Bohr straggling, 16keV detector resolution,
screened Rutherford scattering, pileup, SRIM 2003, multiple &
double scattering)



Same as previous, but with double scattering and pileup

SIMNRA & DataFurnace
almost indistinguishable



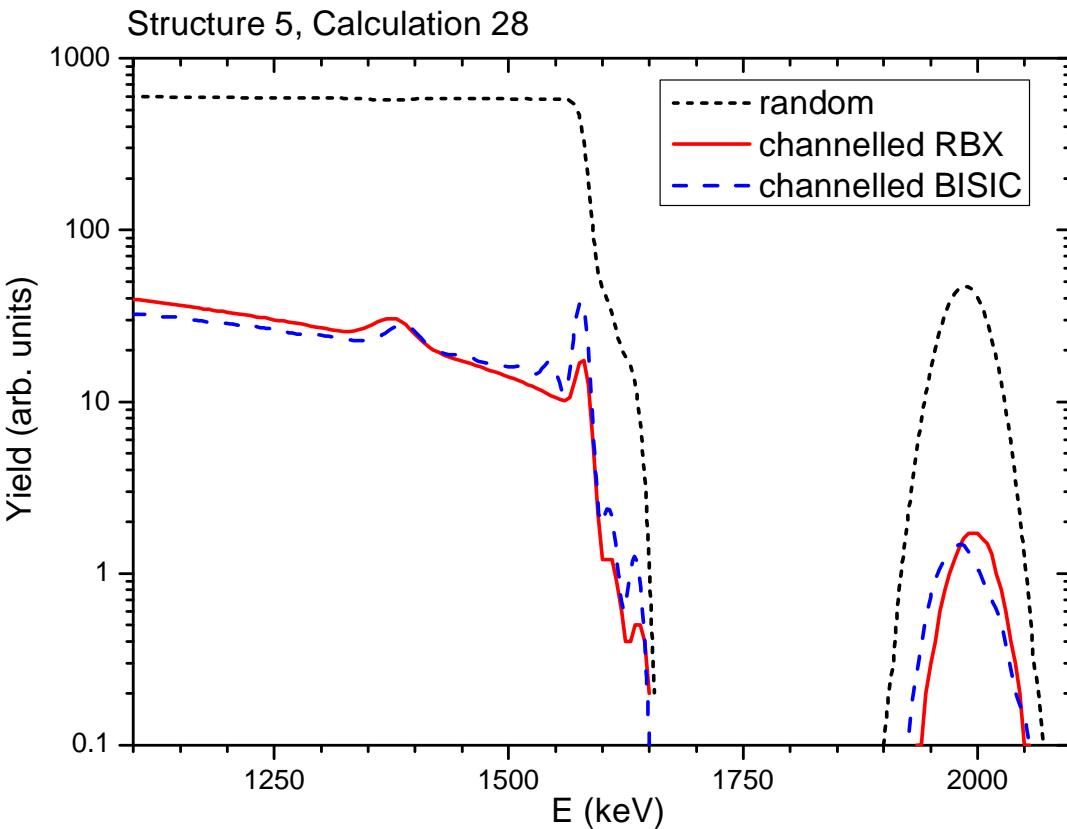
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Simulation of Channelling

100% substitutional 66keV 10^{16} Ge/cm² implant into bulk (100)Si; Si point defect distribution = Ge distribution but with 2% max concentration, Perfect (unreconstructed) surface



Only RBX

Comparison with Monte Carlo code *BISIC* is impressive



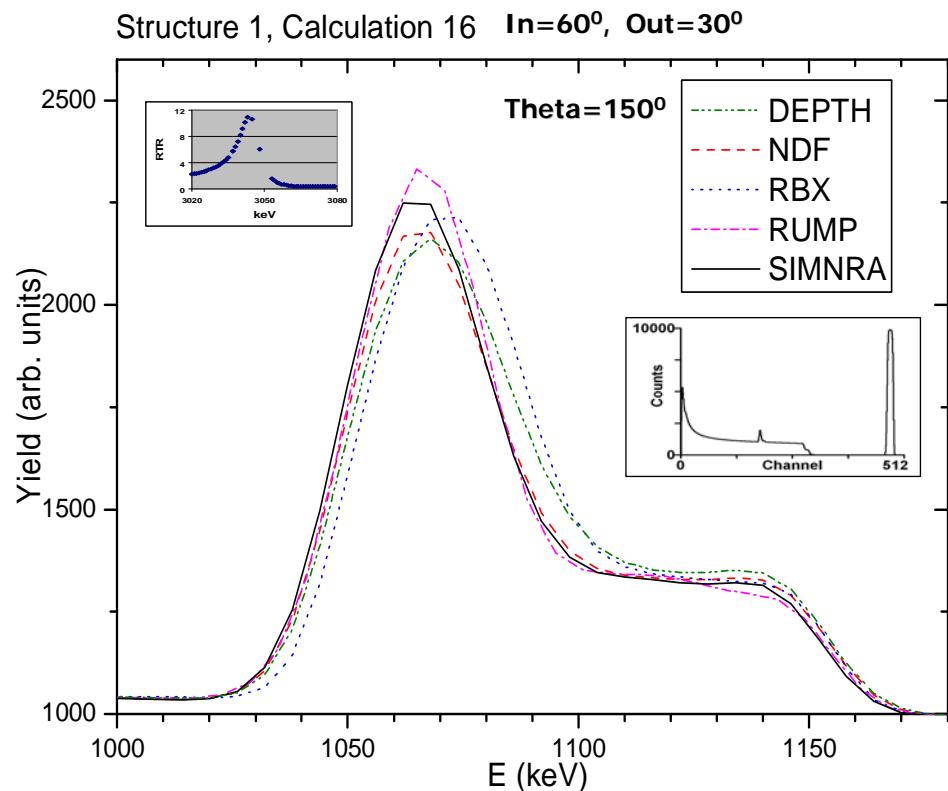
BISIC: E. Albertazzi, M. Bianconi, G. Lulli, R. Nipoti, M. Cantiano, Nucl. Instrum. Methods B118 (1996) 128

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EBS with sharp resonances

Simulation of 50nm Au/200nm SiO₂/Si
3.15 MeV ⁴He⁺, Bohr straggling, SigmaCalc cross-sections for O(α,α)O.



3043keV resonance:
10* Rutherford

4% agreement between
SIMNRA, DataFurnace,
RUMP in region of sharp
resonance

Significant algorithmic
differences: DataFurnace
algorithm demonstrably
superior



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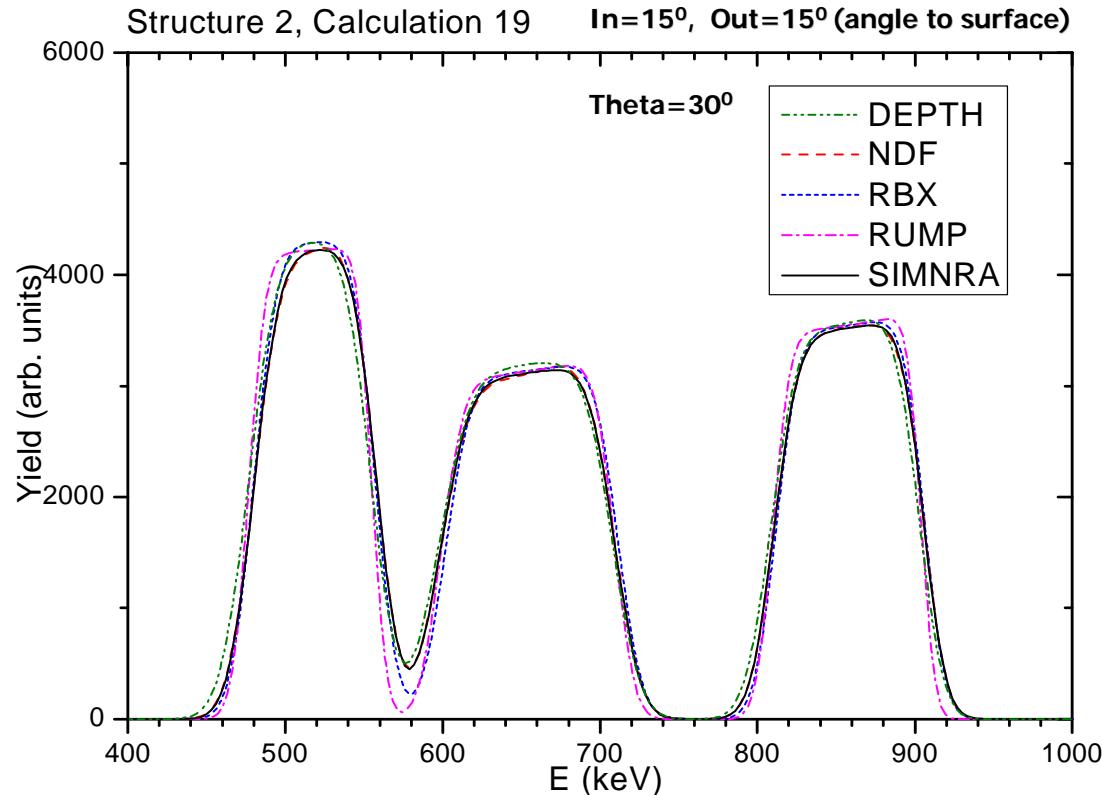
N.P. Barradas, E. Alves, C. Jeynes, M. Tosaki, Nucl. Instrum. Methods B247 (2006) 381-389
A.F. Gurbich, C. Jeynes, Nucl. Instrum. Methods B265 (2007) 447-452

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1.8MeV⁴He ERD, SigmaCalc cross sections Simulation of CD₂ 150nm/CH₂ 150nm/CD₂ 150nm

16keV detector resolution, Bohr straggling



6μm mylar range foil

DataFurnace and SIMNRA agree at:

0.1% (yields),
400eV (edge positions)
~800eV (edge widths)

Excellent agreement with MCERD



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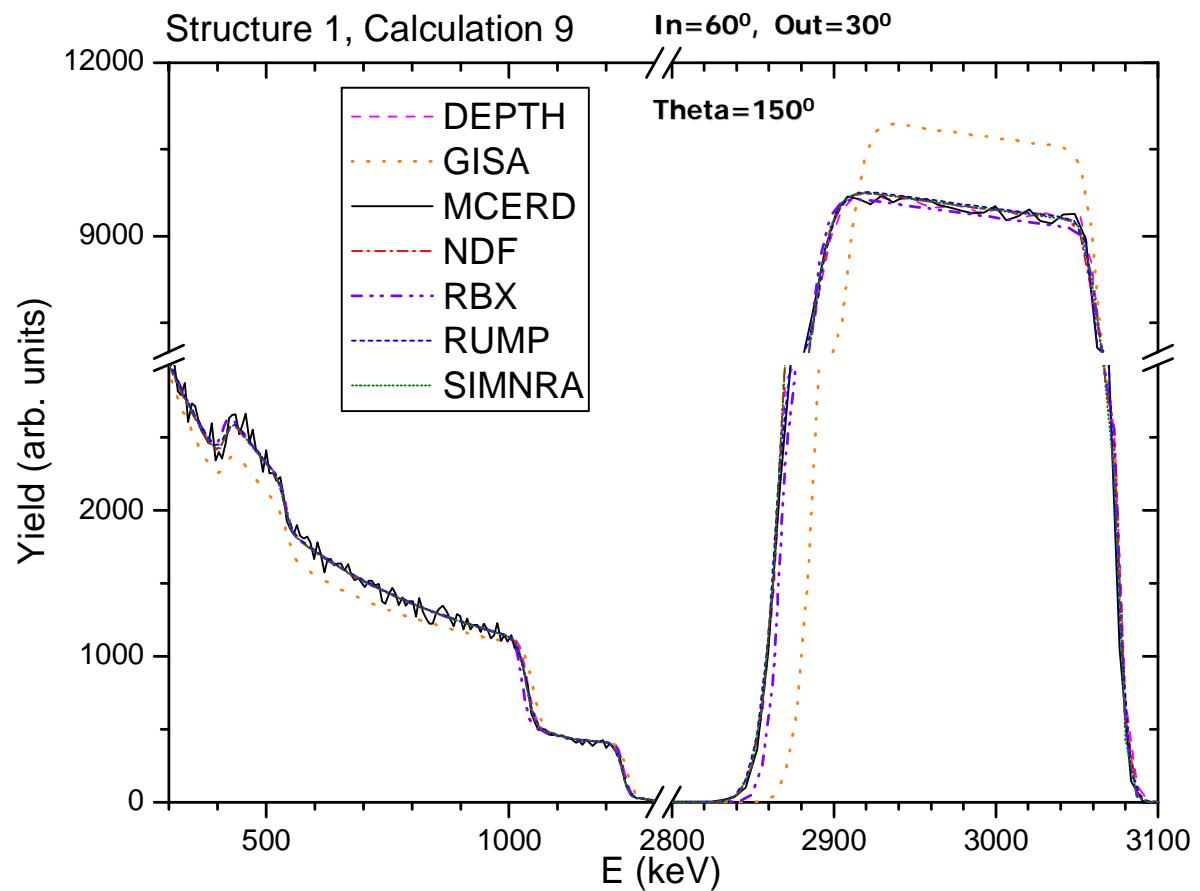
Heavy Ion RBS

Simulation of 50nm Au/200nm SiO₂/Si
(3.5MeV ⁷Li⁺, Bohr straggling, 16keV detector resolution, pure
Rutherford scattering, pileup, SRIM 2003)

GISA: SRIM91

RUMP, SIMNRA,
DataFurnace agree at:
0.3% (Yield/Height)
700eV (edge pos'ns)

SIMNRA, DataFurnace
agree at:
800eV (edge widths)





Heavy Ion ERD

Simulation of 50nm Au/200nm SiO_2/Si
(50MeV $^{127}\text{I}^{10+}$, Bohr straggling, 200keV detector resolution,
SRIM 2003, multiple scattering)



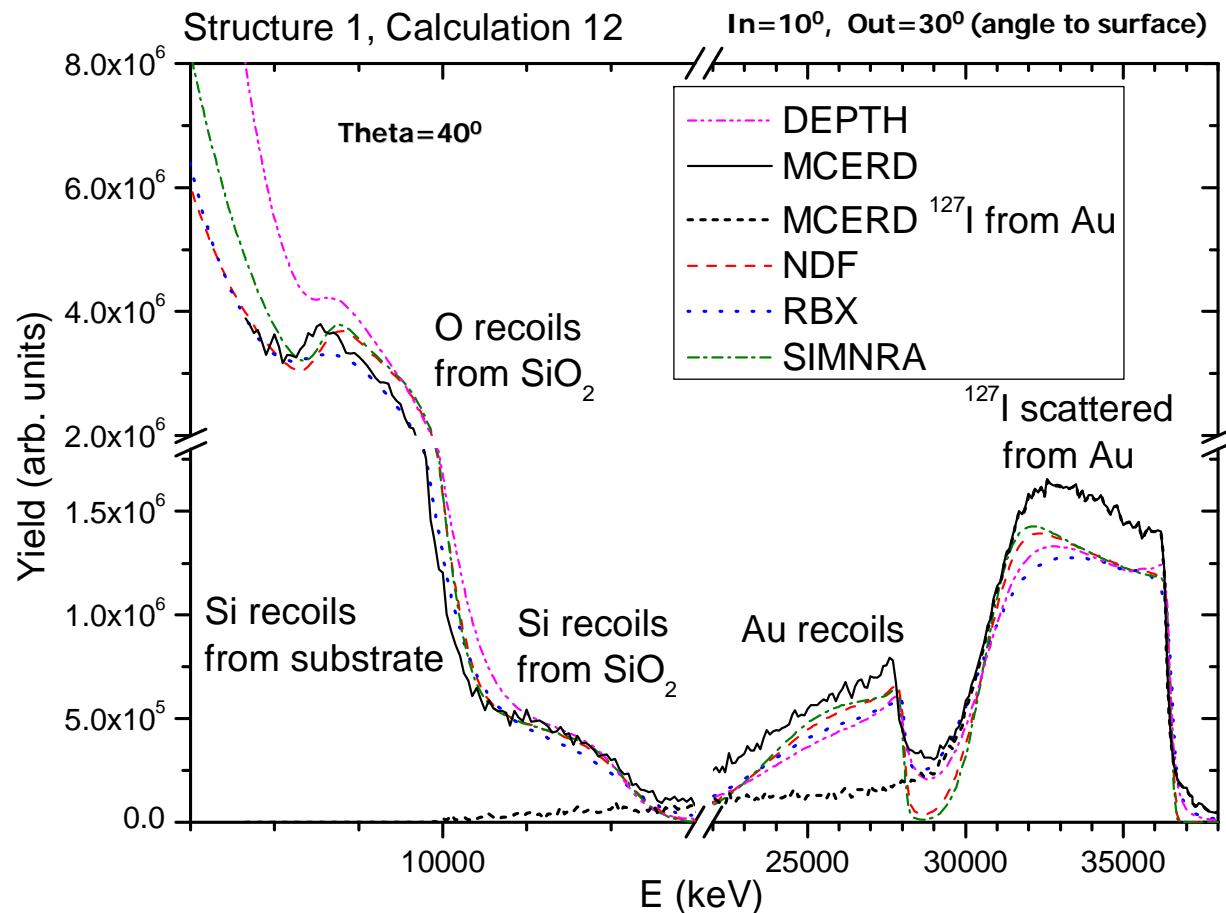
MCERD *not* known
to be good

Analytical codes
appear to have 20%
error on scattered I
signal

Outstanding problem



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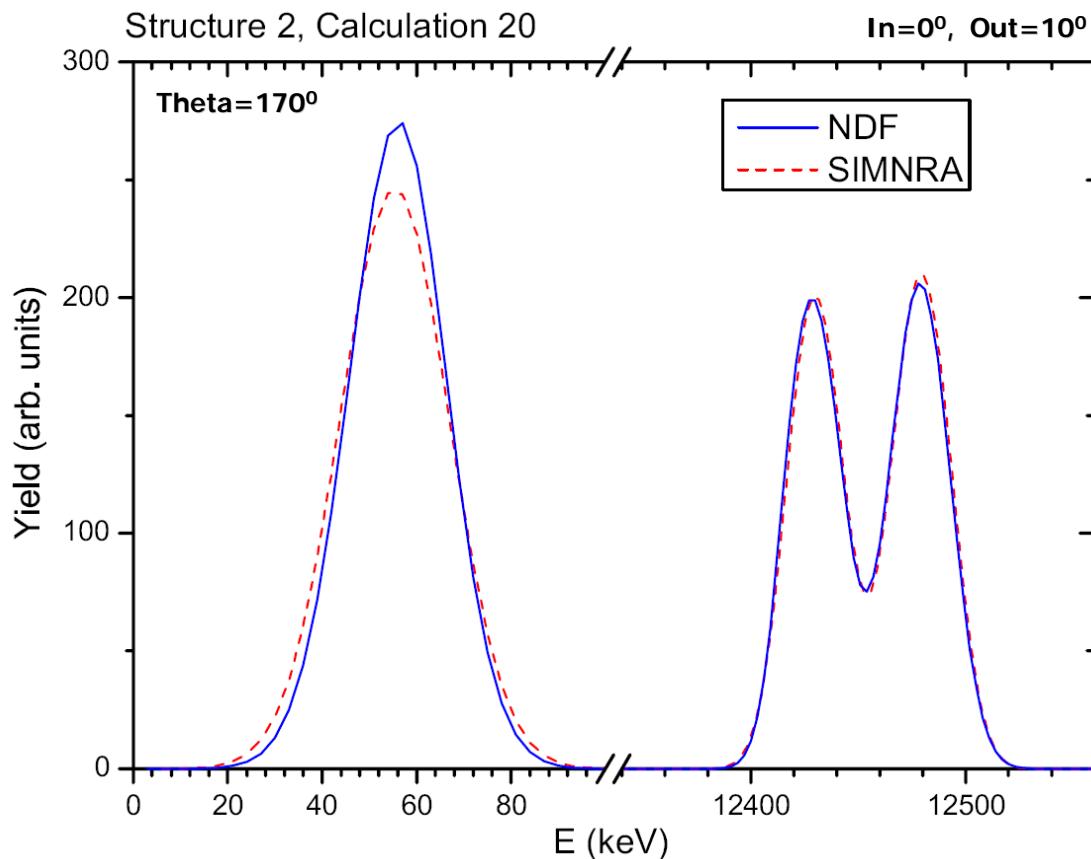


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IMeV³He⁺ NRA

Simulation of CD₂ 150nm/CH₂ 150nm/CD₂ 150nm



d(³He, ⁴He)p

d(³He, p)⁴He

Q=18.35MeV

1980 cross-sections

6um range foil

Low energy (⁴He) signal hard to calculate. NDF carries calculation to lower energies

Excellent agreement for p
signal



W. Möller and F. Besenbacher, Nucl. Instr. and Meth. 168 (1980) 111

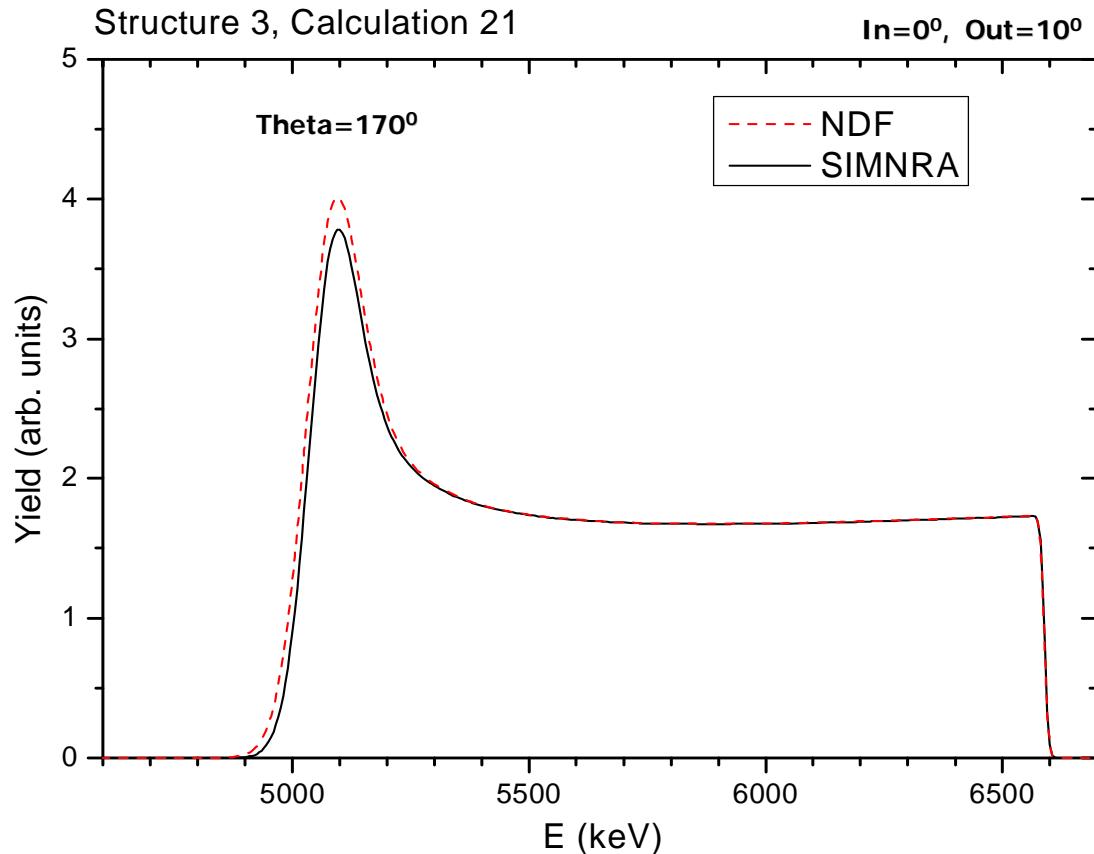
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1MeV²H⁺ NRA

Simulation of a bulk Fe₄N sample



$^{14}\text{N}(\text{d},\text{a})^{12}\text{C}$
Q=13.57MeV
1mb/sr

6um range foil

Inverse kinematics below
550keV



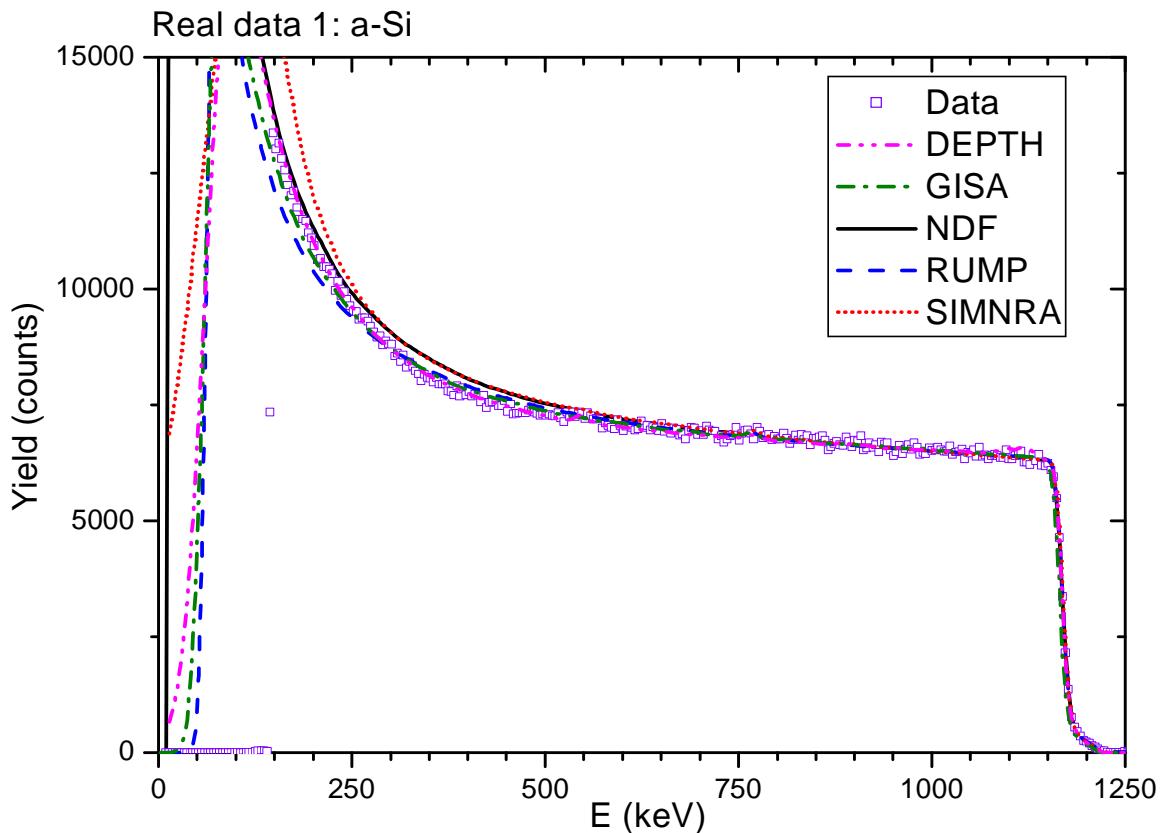
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Real Spectrum of *a*-Si

a-Si, 2MeV, 3.840(8)keV/ch, 1.95(2)msr, 150.0(2) $^{\circ}$
scattering angle, 46.0(5)uC



“... all the codes obtain excellent agreement in the important high energy region of the Si signal”



G. Lulli, E. Albertazzi, M. Bianconi, G.G. Bentini, R. Nipoti, R. Lotti, Nucl. Instrum. Methods B170 (2000) 1.

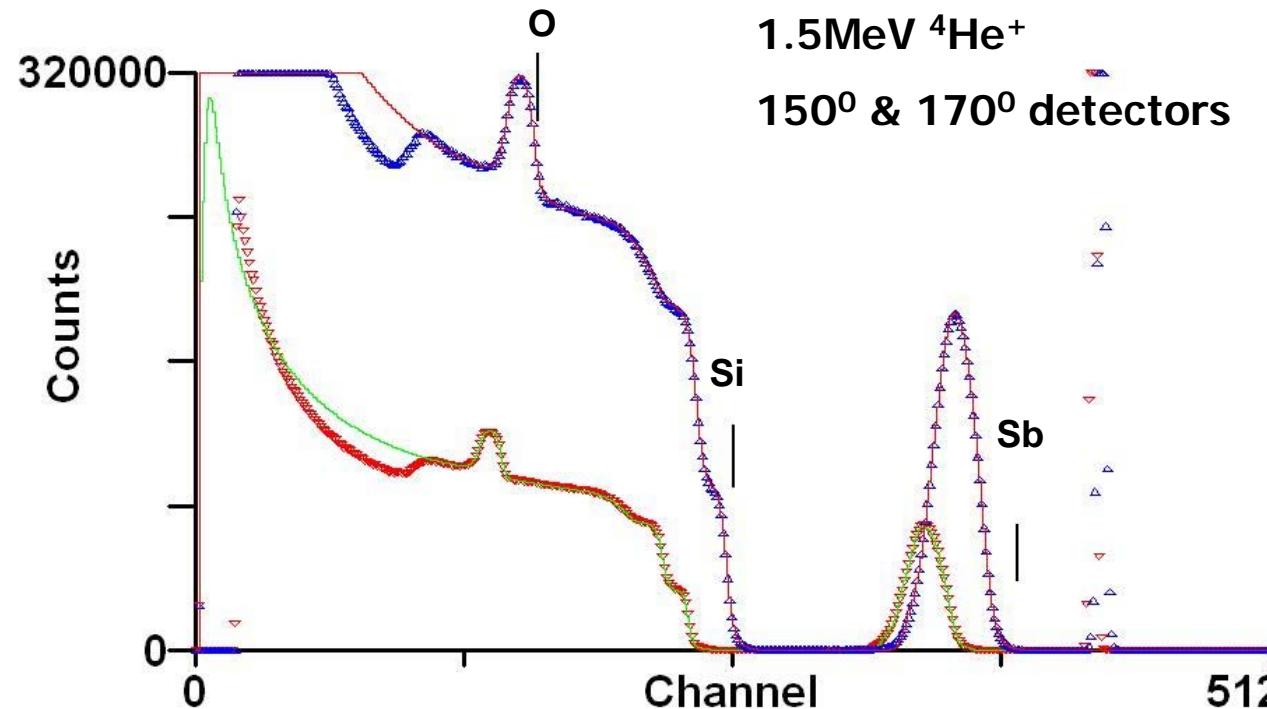
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Real Spectra of Certified Implant

481(3). $10^{13}/\text{cm}^2$ Sb implant in 90nm oxide/a-Si/c-Si



Counting statistics:
0.05%

Gain uncertainty: 0.3%

Total experimental
uncertainty (excluding
stopping): 0.8%

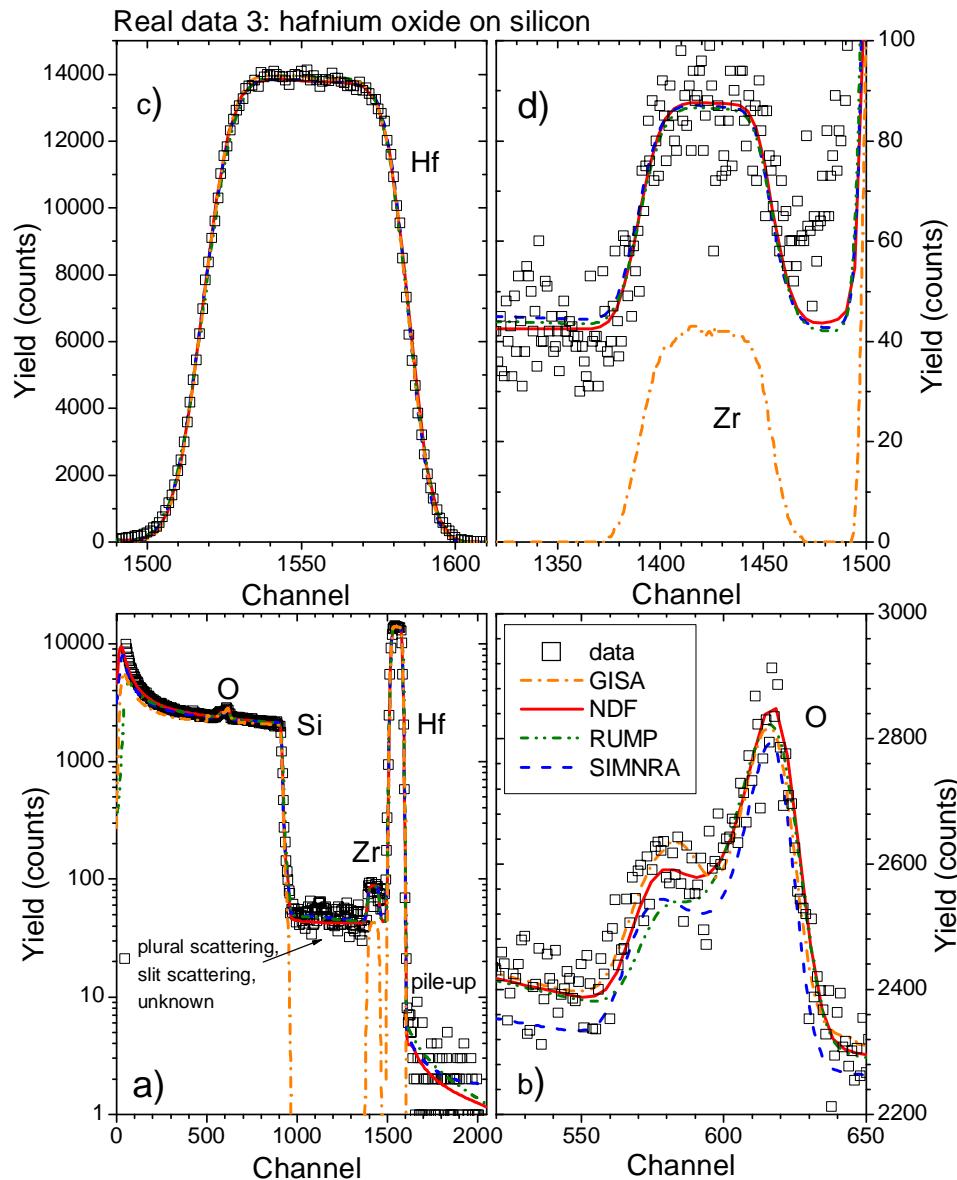
K. H. Ecker, U. Wätjen, A. Berger, L. Persson, W. Pritzcow, M. Radtke, H. Riesemeier, Nucl. Instrum. Methods B188 (2002) 120



Sb fluence determined using SRIM 2003 stopping:
481.15(55). $10^{13}/\text{cm}^2$ (0.1%)

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SigmaCalc cross-sections for O
(2*Rutherford at 2.5MeV)

Assuming HfO_x result is:
 $296(4) \times 10^{15}$ Hf/cm²
 $599(5) \times 10^{15}$ O/cm²

$2.96(8) \times 10^{15}$ Zr/cm²

Uncertainty consistent with
counting statistics



Si bulk / Re 5nm/(Co 2nm/Re 0.5 nm)₁₅

1 MeV ^4He RBS, 160° scattering, 15 keV

Average layer thickness

DataFurnace:

$$356(30) \cdot 10^{13} \text{ Re/cm}^2$$
$$207(17) \cdot 10^{14} \text{ Co/cm}^2$$

SIMNRA:

$$368(31) \cdot 10^{13} \text{ Re/cm}^2$$
$$227(13) \cdot 10^{14} \text{ Co/cm}^2$$

Average layer thickness difference
(normalised)

28pm for the Re layers and
94pm for the Co layers

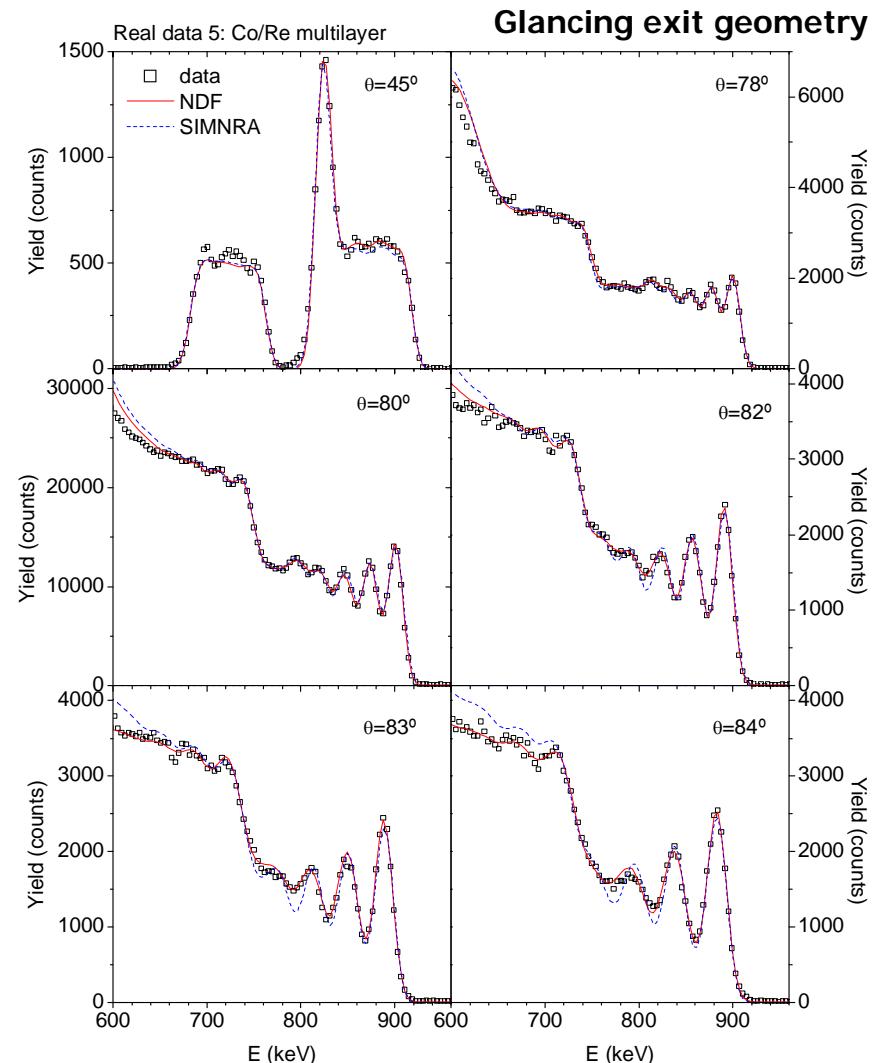
Roughness in conformal layers equivalent
to features 0.6nm high and 40nm wide



N.P. Barradas, J.C. Soares, M.F. da Silva, F. Pászti, and E. Szilágyi, Nucl. Instrum. Methods B 94 (1994) 266 ;

N.P. Barradas, Nucl. Instrum. Methods B190 (2002) 247

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Conclusions (I)

- All codes perform to design
- New generation codes (*DataFurnace & SIMNRA*)
 - Simulation results usually almost *indistinguishable*
 - Excellent results for RBS, HI-RBS, ERD (also RUMP)
 - Excellent results for EBS
 - Excellent results for NRA (including inverse kinematics)
 - Fair results for HI-ERD (also RBX)
 - Roughness and double scattering approximated
 - Accurate pileup (good in RUMP)
- MCERD comparison
 - Need MC code for HI-ERD!
 - MC code is completely independent algorithmically
 - Equivalent results from MC code validates analytical codes
- Summary
 - All codes give reasonable results
 - For HI-ERD you need MCERD
 - For channelling you need RBX (or a Monte Carlo code)
 - Otherwise, for *best* results you need DataFurnace or SIMNRA





Conclusions (II)



- Code validation: 0.1% agreement at best
- SIMNRA and DataFurnace are usually indistinguishable
- Independent implementation of same algorithms
- Independent algorithms (MCERD) also agree
- Incidental demonstration that SRIM03 stopping powers are (accidentally) **correct** (at 0.6%) for 1.5MeV ${}^4\text{He}$ on Si (best stopping powers are currently known at only 2%)
- Thanks to IAEA!

*Nuclear Instruments and Methods B262 (2007) 281-303
summary at: Nuclear Instruments and Methods B266 (2008) 1338-1342*



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<http://www.mfa.kfki.hu/sigmabase/ibasoft/>

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