# Overview of Nuclear and Atomic data in Ion Beam Analysis

Presented by

I. C. Vickridge

Groupe de Physique des Solides
CNRS et Universités de Paris 6 et 7

# Course Objectives

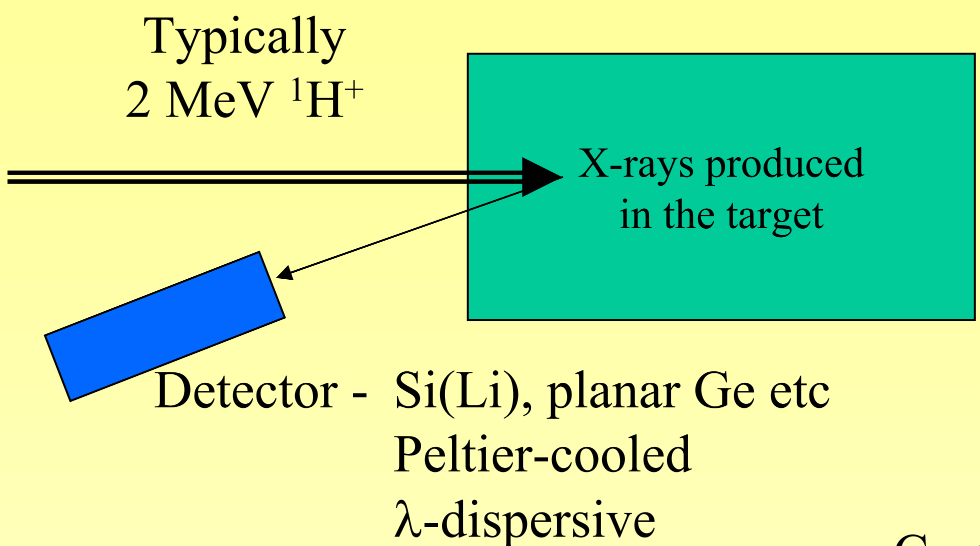
Gain a sufficient understanding of the main IBA methods to understand the requirements for Nuclear (and other) Data

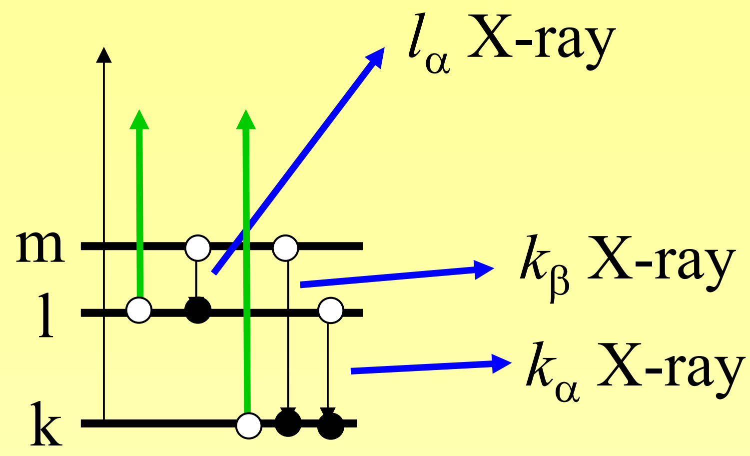
Know how to access and use the main data sources required

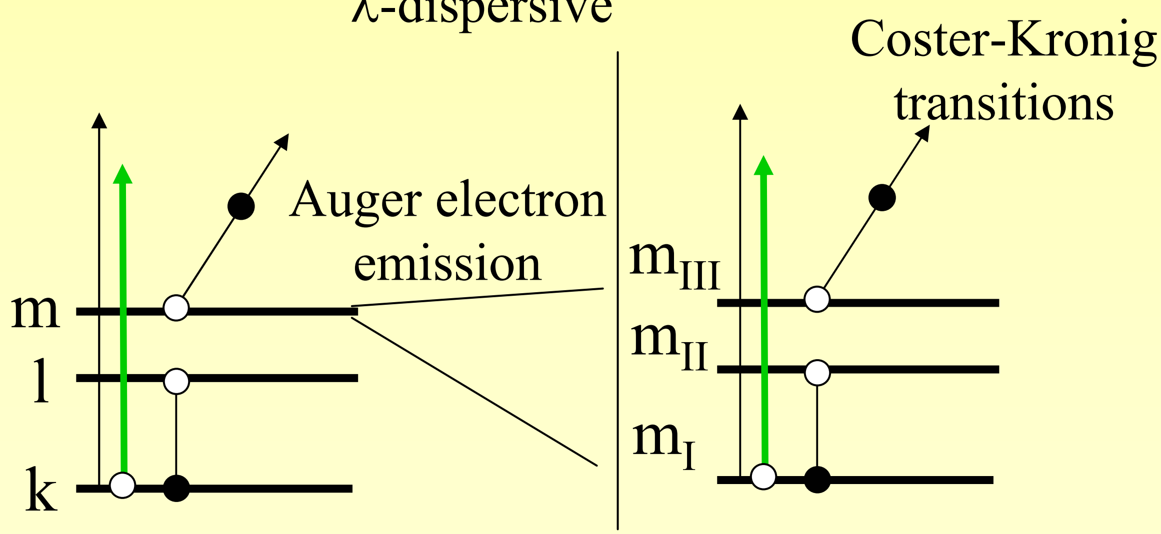
# IBA Methods

| Acronym | | Interaction |
|---|---|---|
| **PIXE** | **P**article-**I**nduced **X**-ray **E**mission | Characteristic X-ray emission following ionization by the primary beam. |
| **PIGE** | **P**article-**I**nduced **G**amma **E**mission | Prompt gamma emission during ion beam irradiation |
| **RBS** | **R**utherford **B**ackscattering **S**pectrometry | Elastic scattering at backward angles |
| **NRA** | **N**uclear **R**eaction **A**nalysis | Nuclear reaction between incident beam and nuclei in the target, producing a light charged particle. |
| **NRP or r-NRA** | **N**uclear **R**esonance **P**rofiling, **r**esonant **N**uclear **R**eaction **A**nalysis | Exploitation of narrow nuclear resonances via scanning of the incident beam energy. |
| **ERDA or FRS** | **E**lastic **R**ecoil **D**etection **A**nalysis, **F**orward **R**ecoil **S**pectroscopy | Elastic recoil at forward angles, not necessarily Rutherford |

# PIXE - Principle




Inner shell ionisation by the incident particle

Characteristic X-ray emission
-> element identification

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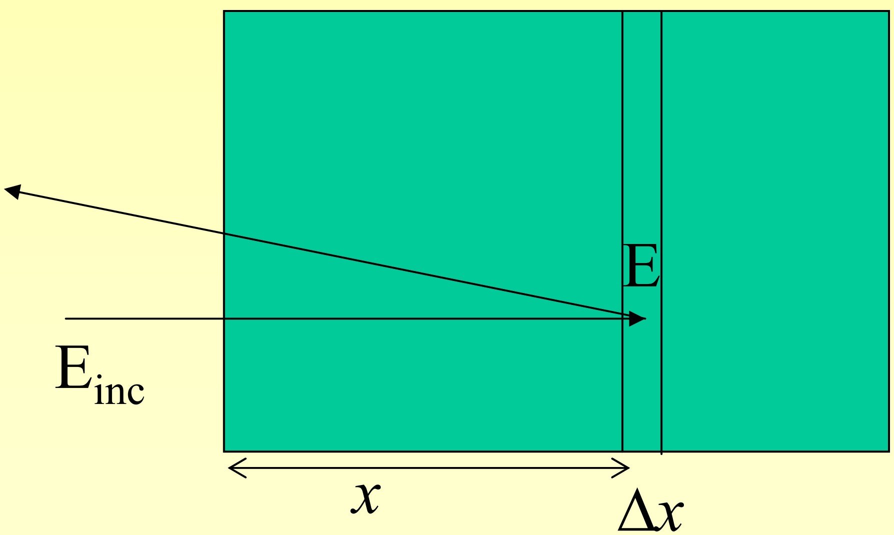
# PIXE Yield from a (buried) thin layer

$$Y_{\Delta x} = N\sigma^{x}(E)e^{(-\mu x)}$$
$$= N\sigma^{i}(E)\omega k e^{(-\mu x)}$$
$$= C\Delta x \sigma^{i}(E)\omega k e^{(-\mu x)}$$
$$= \int_{\Delta x} C(x)\sigma^{i}(E)\omega k e^{(-\mu x)} dx$$




$Y_{\Delta x}$= yield per incident particle

$N$ = number of atoms of the element cm$^{-2}$ in Δx

C=element concentration cm$^{-3}$

$\sigma^{x}$= x-ray production cross section

$\sigma^{i}$= ionisation cross section

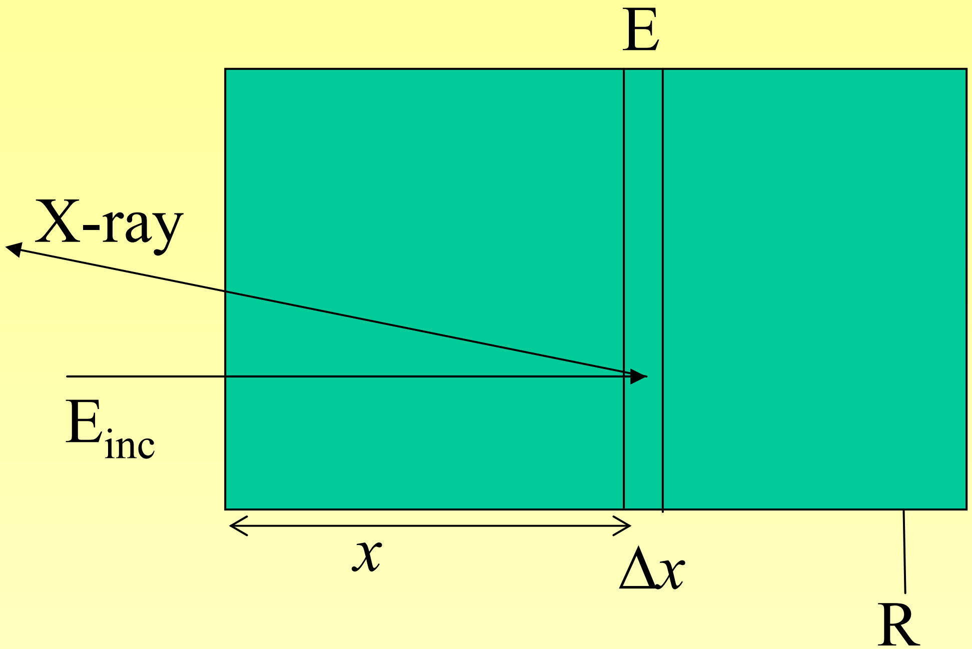
$\mu$ = mass attentuation coefficient

$t$ = depth

$\omega$=fluorescent yield

$k$= relative transition probability

# PIXE yield from a thick target




$$Y = \int_0^R C(x)\sigma^i(E)\omega k e^{(-\mu x)}dx$$

$$= \omega k \int_{E_{inc}}^0 \frac{C(x(E))\sigma^i(E)e^{(-\mu x(E))}}{S(E)}dE$$

$$\left(\text{using } S(E) = \frac{dE}{dx}\right)$$

$$x(E) = \int_{E_{inc}}^0 \frac{1}{S(E)}dE - \int_E^0 \frac{1}{S(E)}dE$$

$$= R_{E_{inc}} - R_E$$

Need
- Ionisation cross sections
- Fluorescence yields
- Transition probabilities and Coster-Kronig coefficients
- Mass attenuation coefficients
- Stopping powers

# PIXE Data Needs

Ionisation cross sections

Fluorescence yields

Transition probabilities and Coster-Kronig coefficients

Mass attenuation coefficients

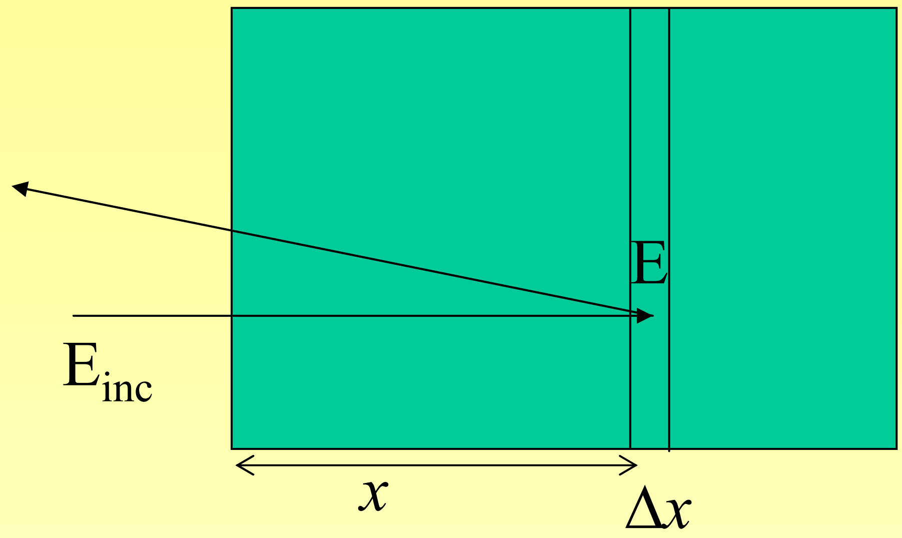
Stopping powers

# PIGE : principle

$$Y_{\Delta x} = N\sigma(E)\, \cancel{e^{(-\mu x)}}$$

$$= C\Delta x \sigma(E)$$

$$= \int_{\Delta x} C(x)\sigma(E)dx$$




$$Y = \int_{x=0}^{R} C(x)\sigma(E)dx$$

$$= C \int_{E=E_{inc}}^{0} \frac{\sigma(E)}{S(E)} dE$$

$$\int_{E=E_{inc}}^{E=0} \frac{\sigma(E)}{S(E)} dE \cong \frac{1}{S} \int_{E=E_{inc}}^{E=0} \sigma(E) dE$$

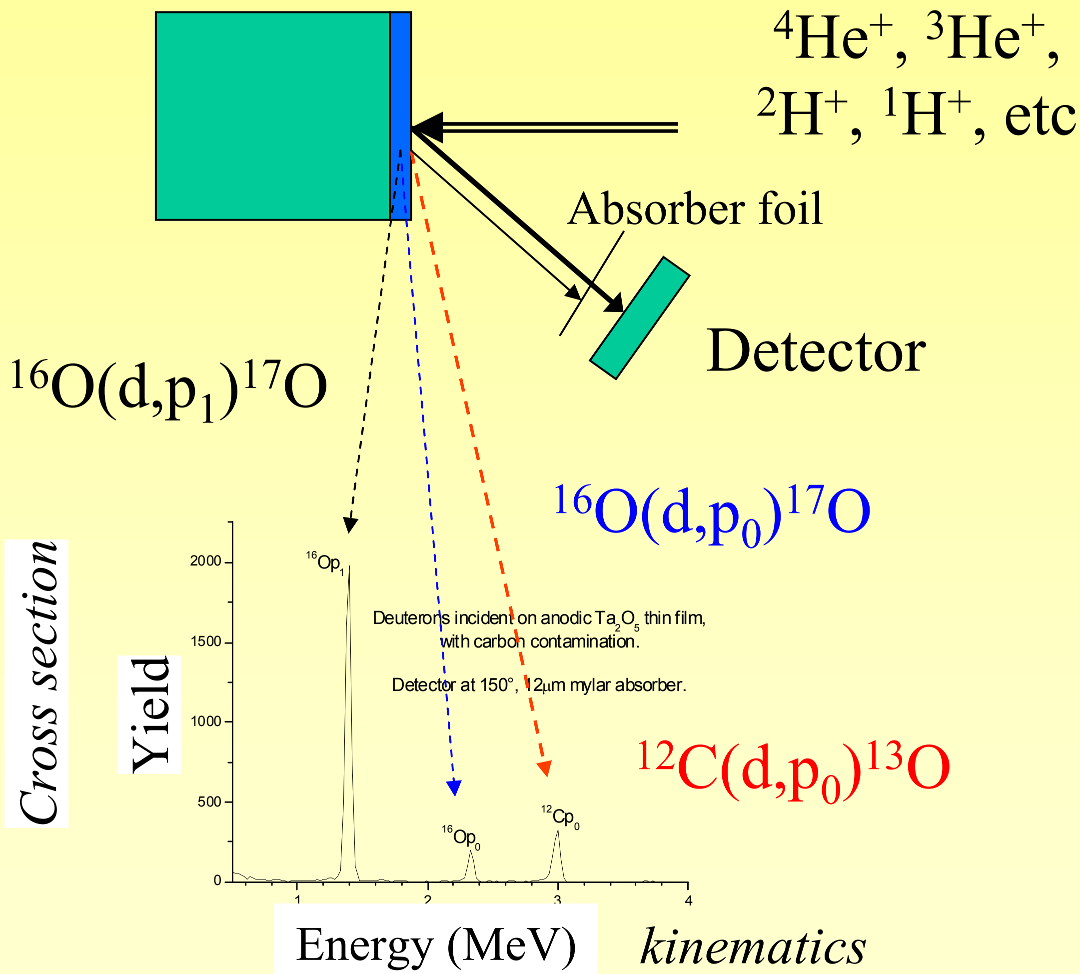
$$S = S(E_{1/2}) \text{ or } S = S(E_{inc})$$

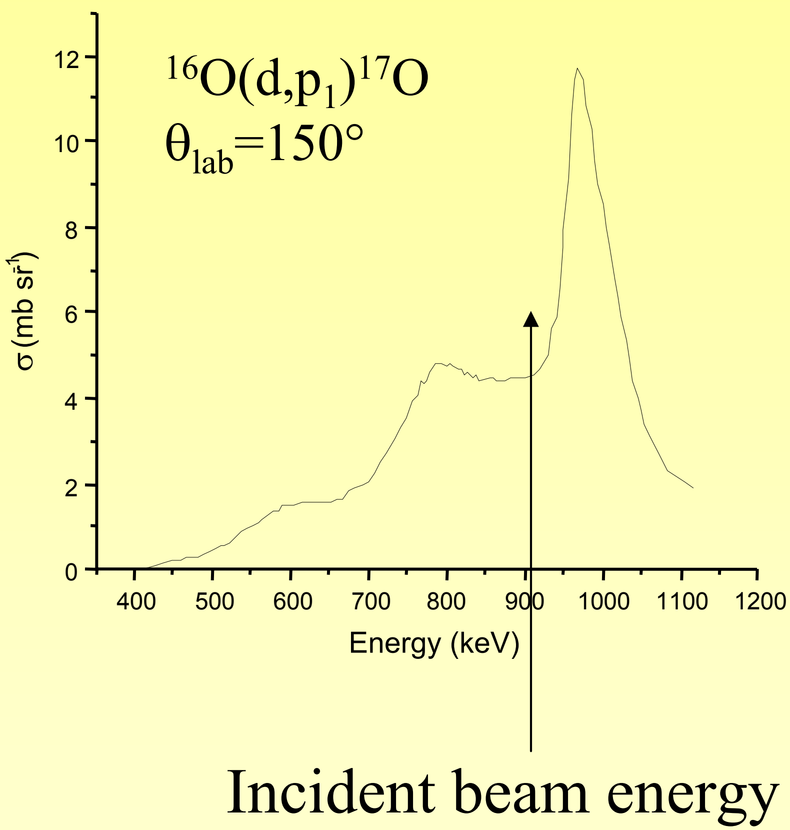
# PIGE Data needs :

- Accurate stopping powers
- Low priority need for σ(E) (standardless PIGE?)
- Long term need for centralised library of accessible isotopic PIGE spectra and cross sections

(see libraries of Antilla et al, Kiss et al …)

# NRA Thin Sample Principle



# NRA – Thin sample : quantitation

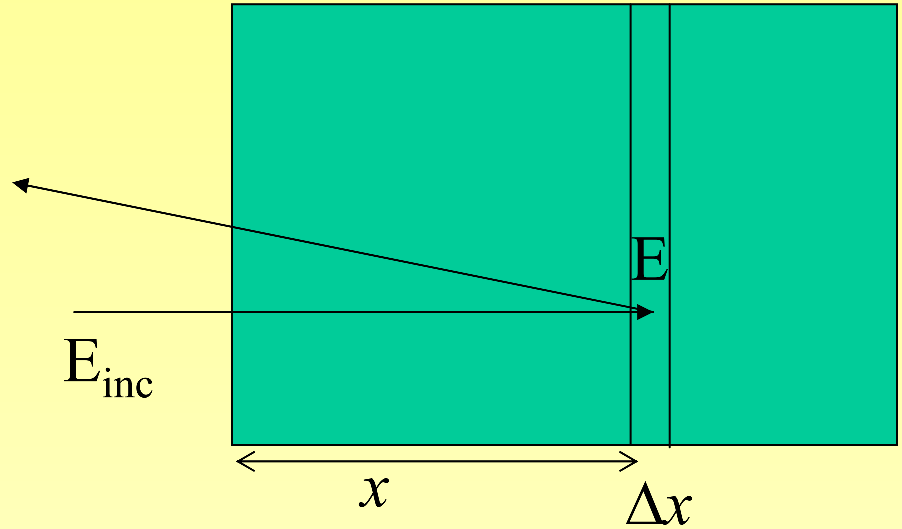
$$Y = N\sigma(E)\,\cancel{e^{(-\mu x)}}$$

$$= C\Delta x\sigma(E)$$

$$= \int_{\Delta x} C(x)\sigma(E)dx$$

$$\Downarrow$$

$$N_U = \frac{Y_U}{Y_R} N_R$$




Y = number of particles detected in peak per incident particle
N= areal density of detected nucleus

# NRA Reference materials

$$N_U = \frac{Y_U}{Y_R} N_R$$

Anodic isotopic $Ta_2O_5$ thin films for $^{16}O$ and $^{18}O$

Certified $^{16}O$ films available from IRMM, Belgium

$^{18}O$ films on special request and subject to availability from I. C. Vickridge

For thin targets, the cross section ratios of $^{12}C(d,p)^{13}C$, $D(^{3}He,p)^{4}He$, $^{14}N(d,\alpha)^{12}C$, $^{14}N(d,p)^{15}N$, $^{15}N(d,\alpha_0)^{13}C$ and $^{15}N(p,\alpha_0)^{12}C$ to that of $^{16}O(d,p_1)^{17}O$ have been obtained by using stoichiometric frozen gas targets of $CO_2$, NO and $D_2O$.

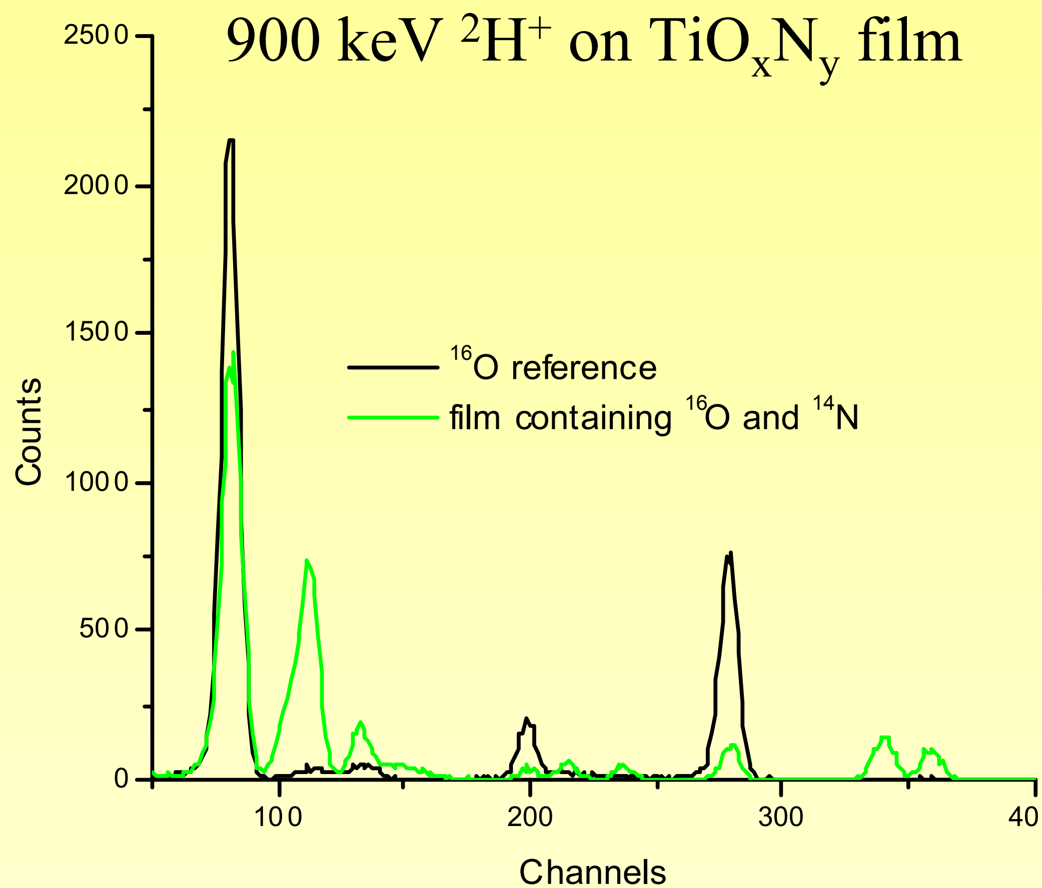
This enables the reliable and robust $Ta_2O_5$ reference targets to be used as a reference for NRA determinations of {D}, {$^{12}C$}, {$^{14}N$} and {$^{15}N$}.


Davies, J. A., T. E. Jackman, et al. (1983). "Absolute calibration of 14N(d,a) and 14N(d,p) reactions for surface adsorption studies." Nucl. Instr. and Meth. **218**: 141-146.

Sawicki, J. A., J. A. Davies, et al. (1986). "Absolute cross sections of the 15N(d,a0)13C and 15N(p,a0)12C reaction cross sections." Nucl. Instr. and Meth. **B15**: 530-534.

# NRA Thin sample : interferences

Numerous overlapping peaks from $^{14}N(d,p_{0-7})$ and $^{14}N(d,\alpha_{0,1})$ reactions.




Reaction Q-values are known

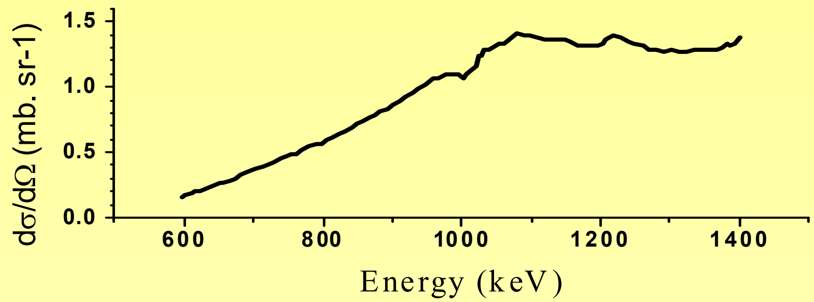
In principle, interferences can be accounted for.
In practice we avoid having to.

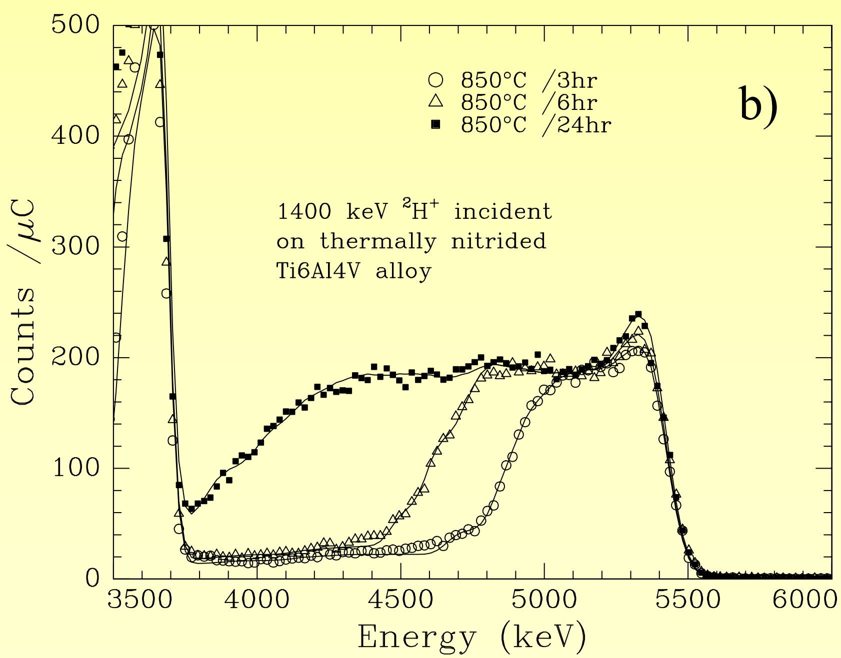
# NRA – Thin sample : summary

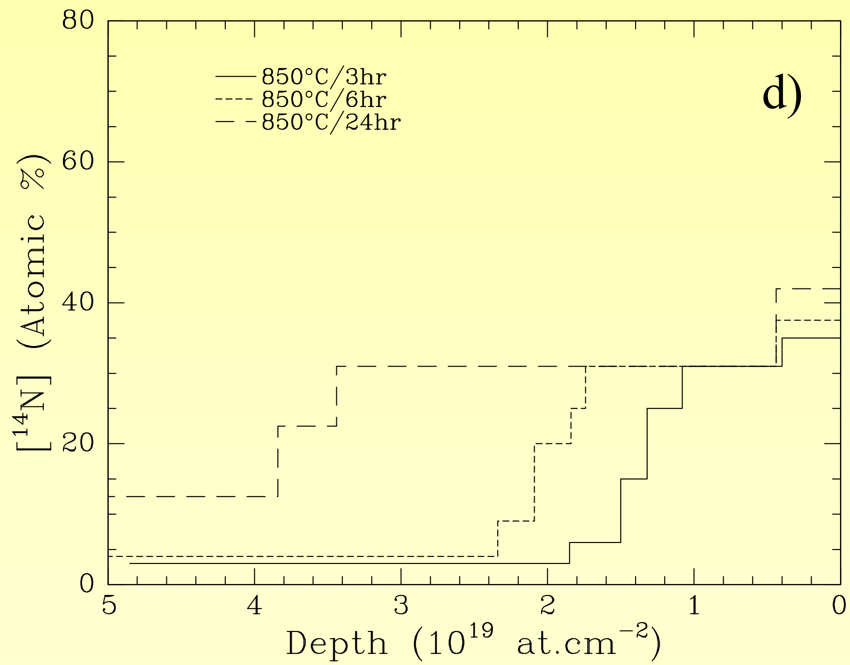
- dE/dx not needed
- Shape of $\sigma(E, \theta)$ much more important than absolute value. Precision standards are used rather than precision cross sections (Standardless NRA?)
- Approximate *relative* cross sections are needed to help in experimental design (isotopes …)
- Reaction Q values are needed - these are easily accessible and well known.

# NRA - depth profiling example

Depth profiling
nitrogen in titanium via
$^{14}N(d,\alpha_1)^{12}C$

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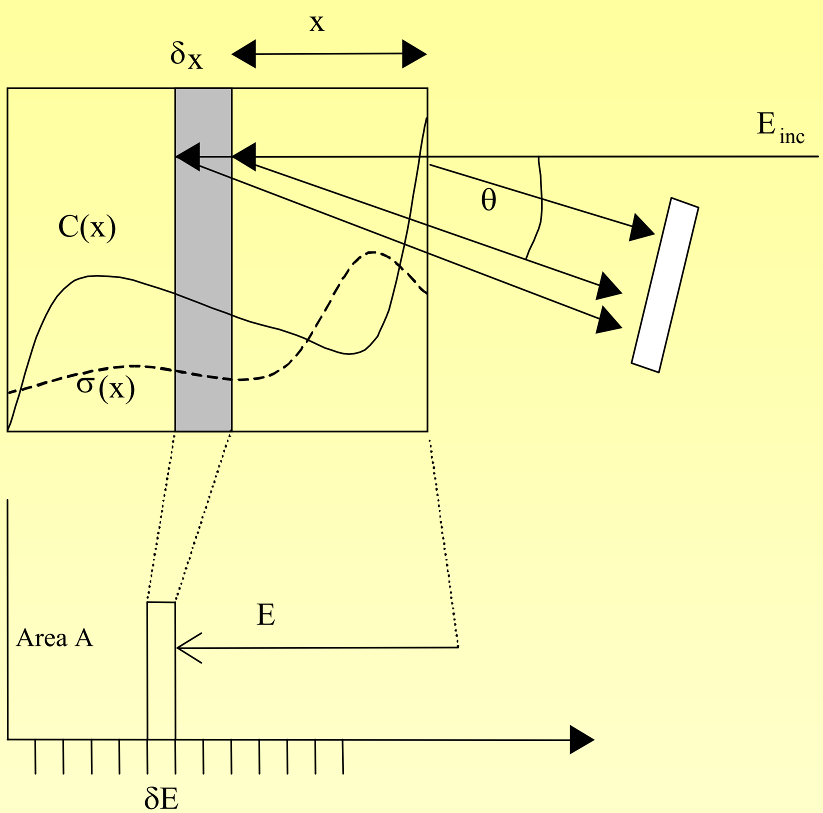
# NRA Depth Profiling : Principle

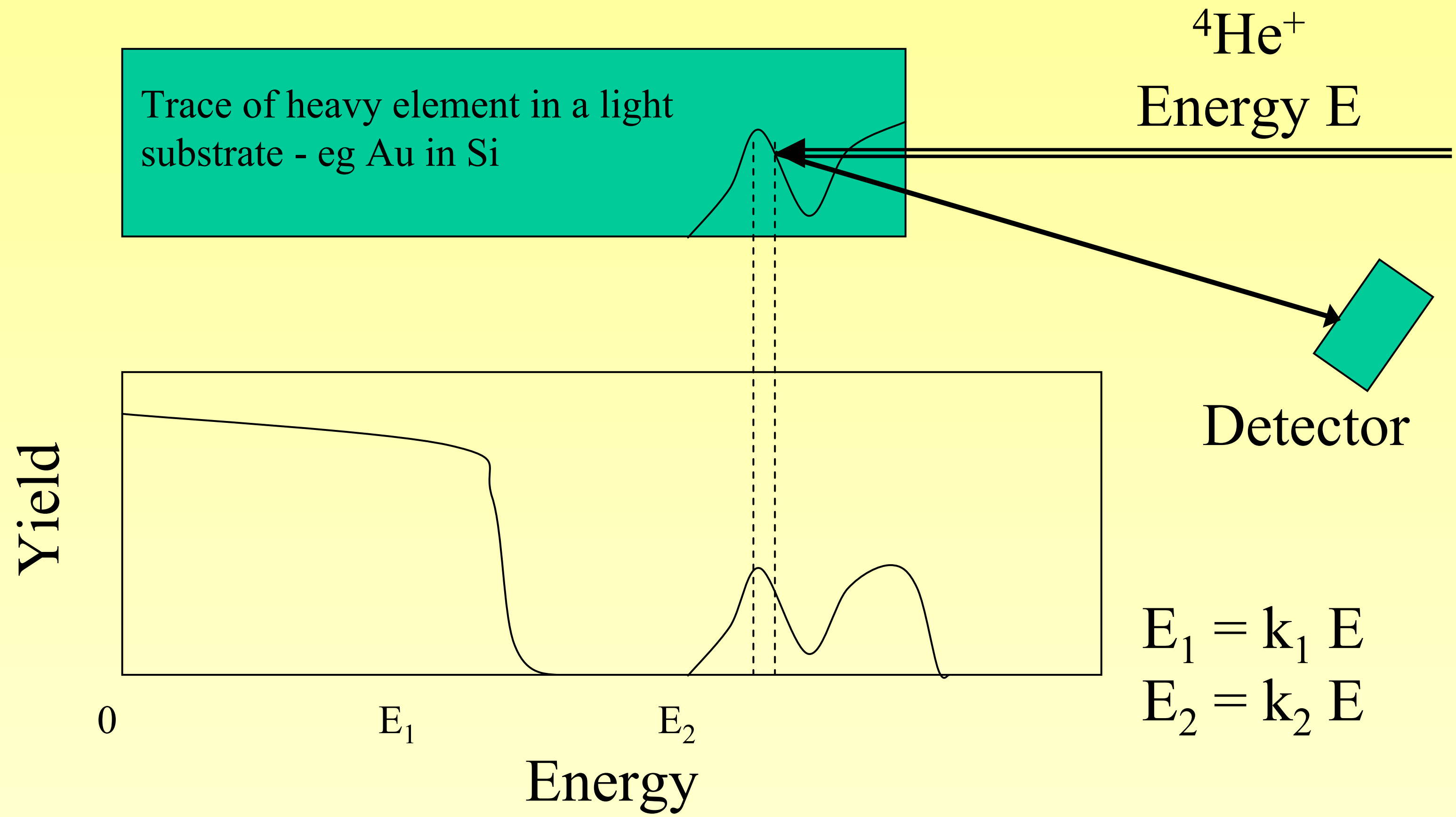



- A channel of width $\delta E_c$ at energy $E_c$ in the spectrum corresponds to a slice of width δx at depth x in the sample, with Ec and δEc being inversely related to x and δx through a linear combination of the stopping powers for the incident and outgoing particle
- The number of particles accumulated into that histogram bin is proportional to C(x), δx, and $\sigma(E_x)$, where $E_x$ is the energy of the incident beam when it gets to depth x;

# NRA Depth Profiling summary

- As for thin samples, plus need for accurate S(E)
- Stronger requirement for shape accurate $\sigma(E,\theta)$ for accurate depth profiling

# RBS - principle

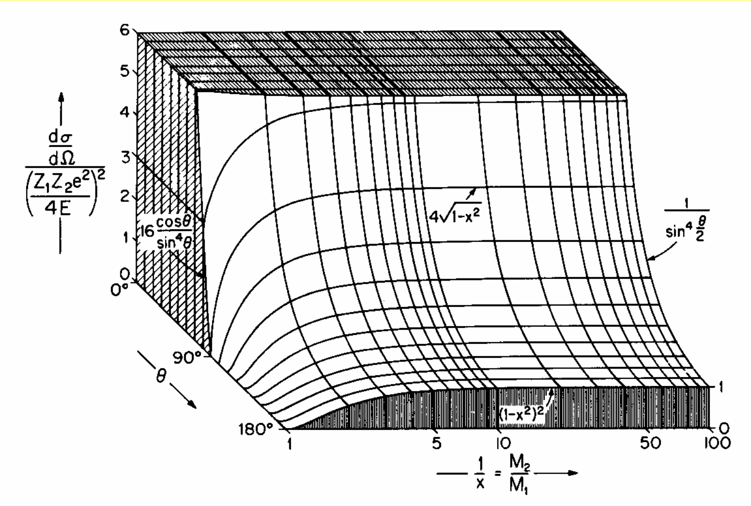



$E_1 = k_1 E$

$E_2 = k_2 E$

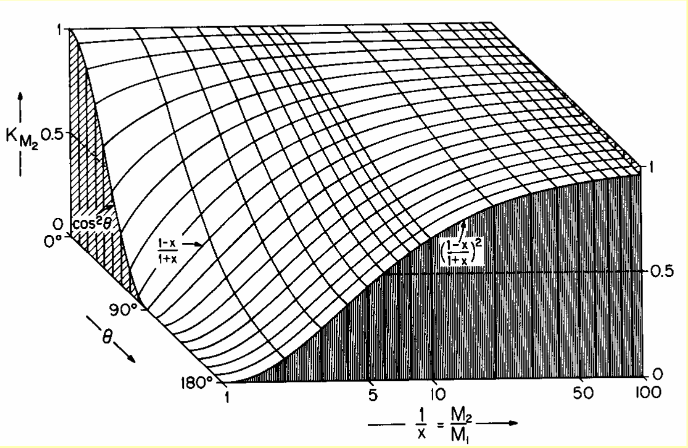
# RBS – Data!

## Rutherford cross section (Coulomb scattering)



Stolen from Backscattering Spectrometry, Chu, Mayer and Nicolet, Academic Press, 1978

## Kinematics

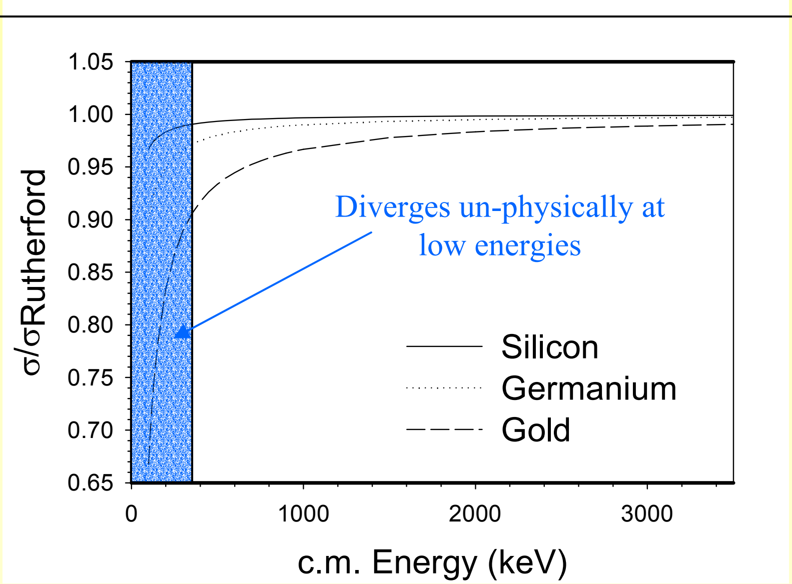


## Screening

L'Ecuyer, Davies and Matsunami, Nucl. Instr. And Meth. 160 (1979) 337

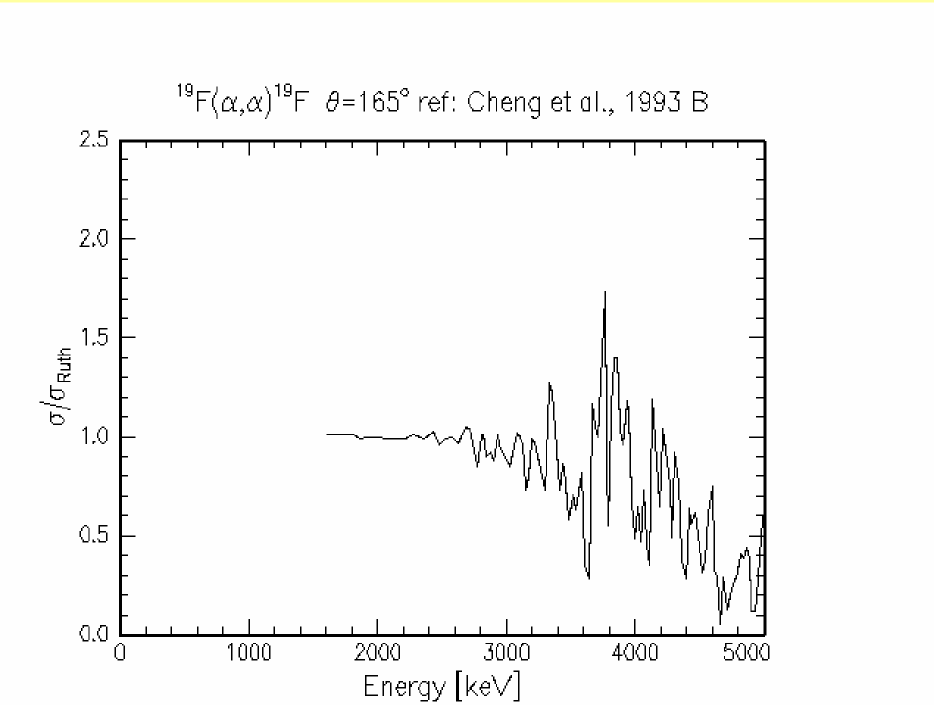
$$\frac{\sigma}{\sigma_{\text{Rutherford}}} = 1 - \frac{0.049 Z_1 Z_2^{4/3}}{E}$$

*See also* Schumann et al. Eur. Phys. J. **A** 2 337-342 (1998)

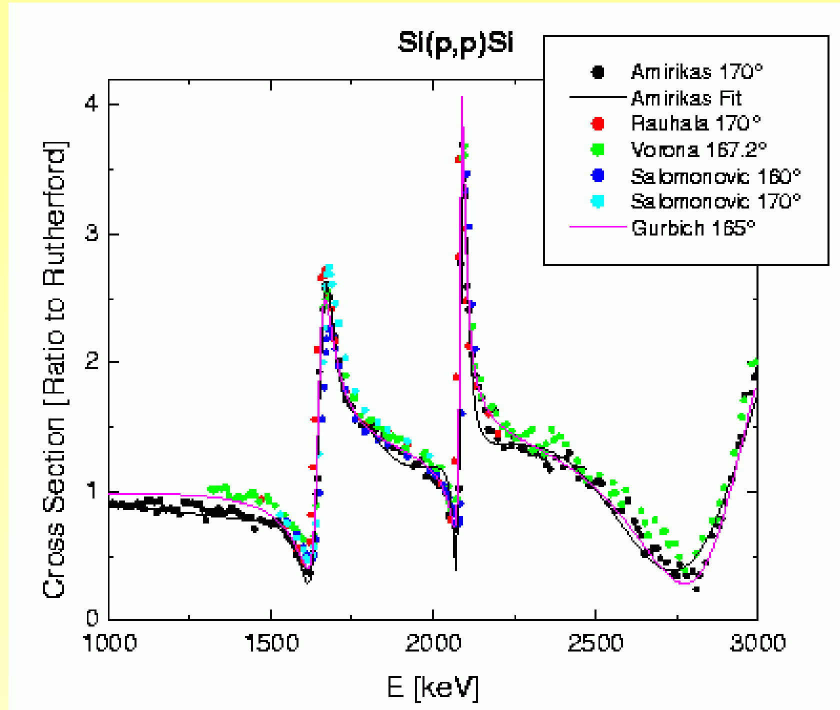


# RBS – non-Rutherford σ(E)

E.g from Sigmabase




E.g from Simnra




Elastic scattering of $^1$H, $^4$He, $^2$H, $^3$He

Resonances, plateaux of enhanced σ(E)

Isotopes … Natural/enriched targets.

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# RBS Data Needs

Accurate Stopping Powers

Accurate Non-Rutherford cross sections

NB: RBS References

Implanted Bi into amorphised Si. {Bi} accurate to about 2% (1$\sigma$)
Available from IRMM.

# Databases for stopping powers and nuclear cross-sections for IBA

**dE/dx**

www.srim.org Doing globally better than Ziegler and coworkers will be a huge task.

See literature for specific cases - e.g. $^4$He in Si

ICRU report 49 (1993), Pstar, Astar

physics.nist.gov/PhysRefData/Star/Text/contents.html

**CP Nuclear reaction and non-Rutherford cross sections**

EXFOR - increasing differential CP cross sections

www.mfi.kfi.hu/sigmabase (some further files also distributed with SimNRA)

- compilation, not formally evaluated

NRABase/SigmaCalc

# PIGE spectra and thick target yields

PIGE : some spectrum libraries and thick target yields are available in the litterature.

Anttila, A., R. Hanninen, et al. (1981). *Proton-Induced Thick-Target Gamma-Ray yierlds for the elemental analysis of the Z=3-9,11-21 elements.* J. Radiaoanal. Chem. **62**(1-2): 293-306

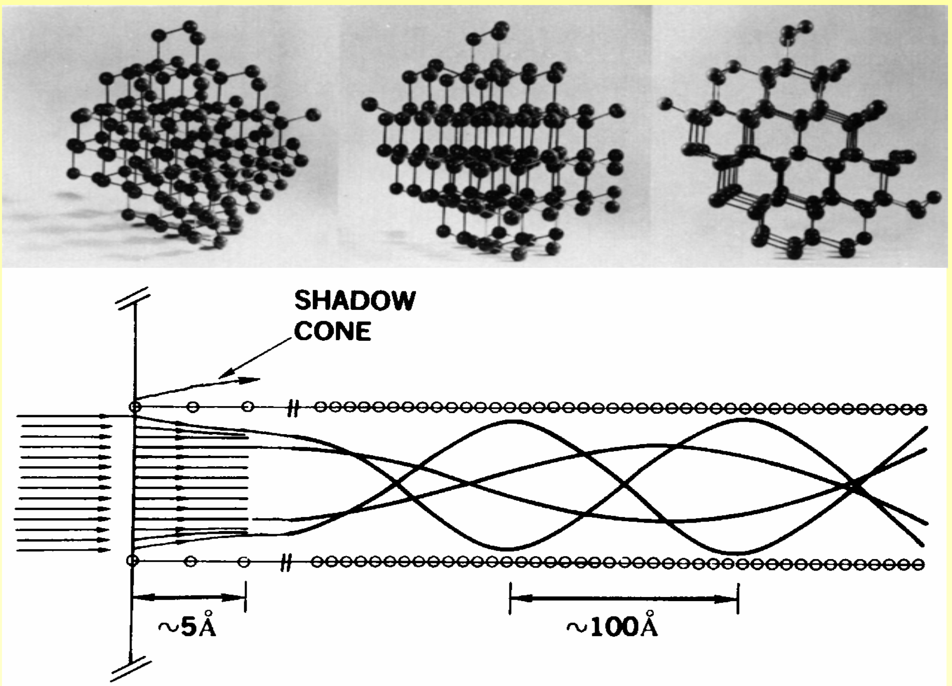
Kiss, A. Z., E. Koltay, et al. (1985). "Measurements of relative thick target yields for PIGE analysis on light elements in the proton energy interval 2.4 - 4.2 MeV." J. Radioanal. and Nucl. Chem., Articles **89**(1): 123-141.

Kiss, A. Z., I. Biron, et al. (1994). "Thick target yields of deuteron induced gamma-ray emission from light elements." Nucl. Instr. and Meth.B 85(1-4) 764-769

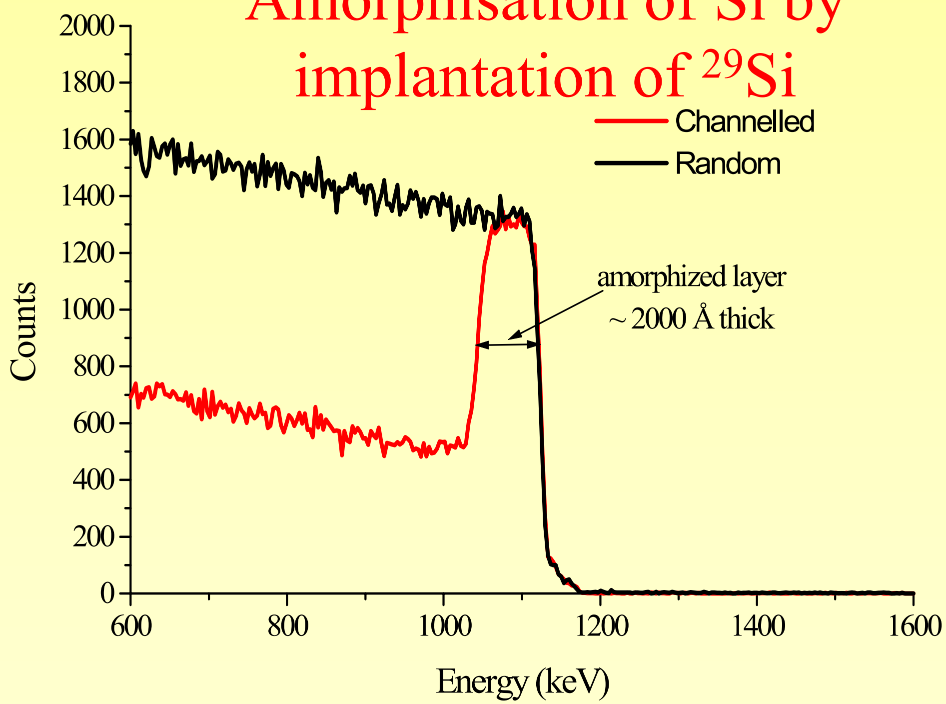
Elekes, Z., Kiss, A.Z. Biron, I. et al. (2000) "Thick target $\gamma$-ray yields for light elements meqsured in the deuteron energy interval of 0.7-3.4 MeV, Nucl. Instr. and Meth.B 168 305-320.

# What we have not talked about

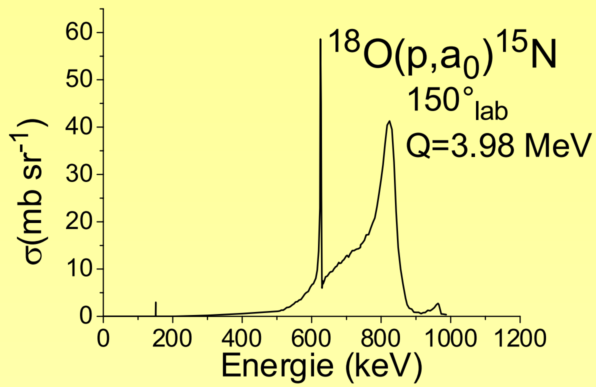
## Ion Channelling



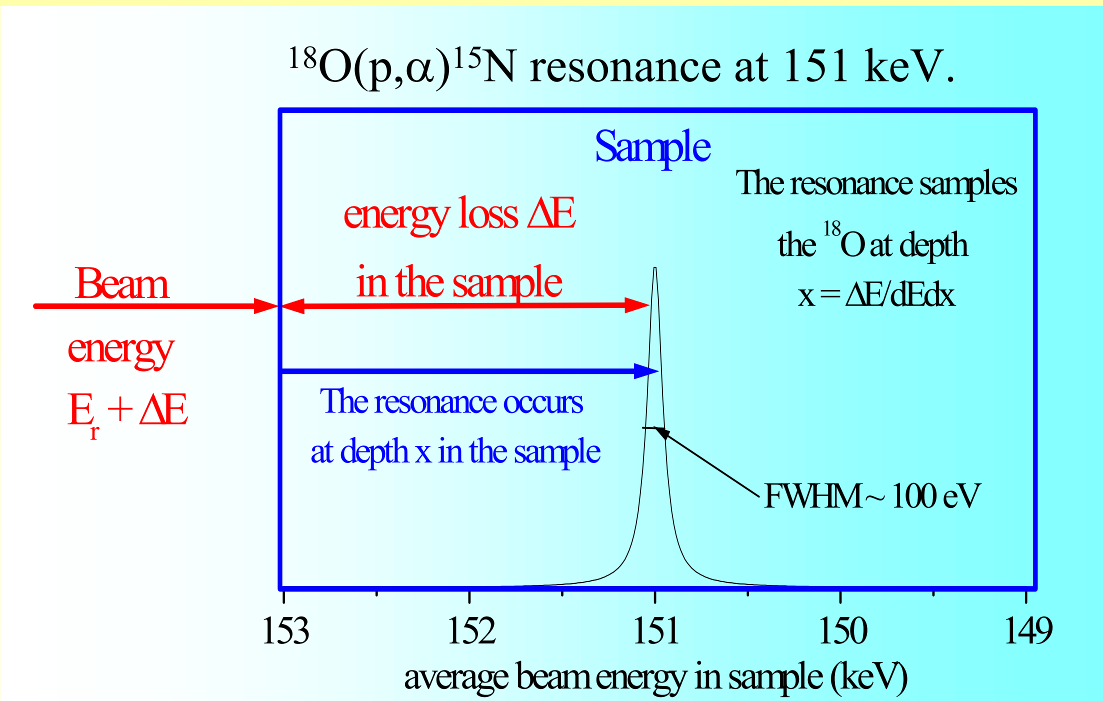

Amorphisation of Si by implantation of $^{29}Si$

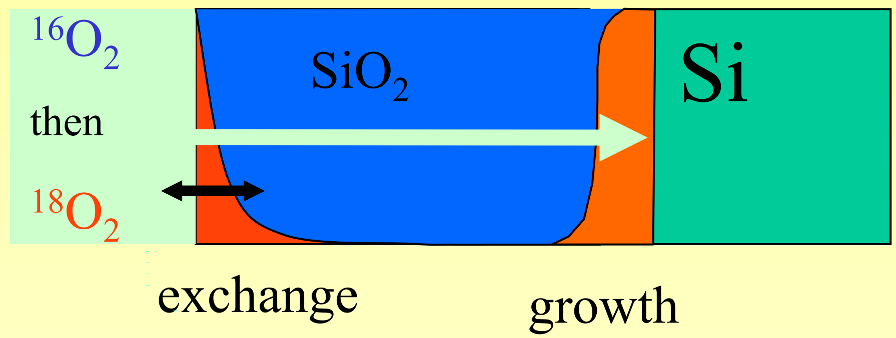


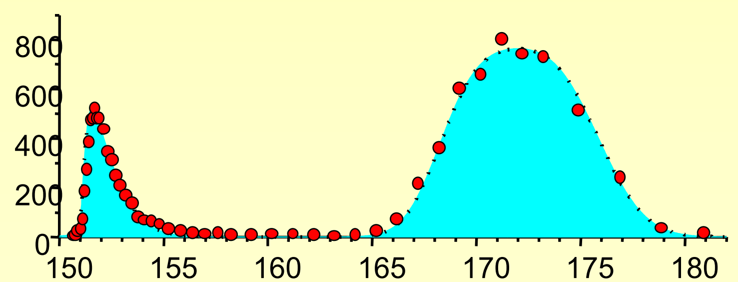
# What we have not talked about




## Nuclear Resonance Profiling

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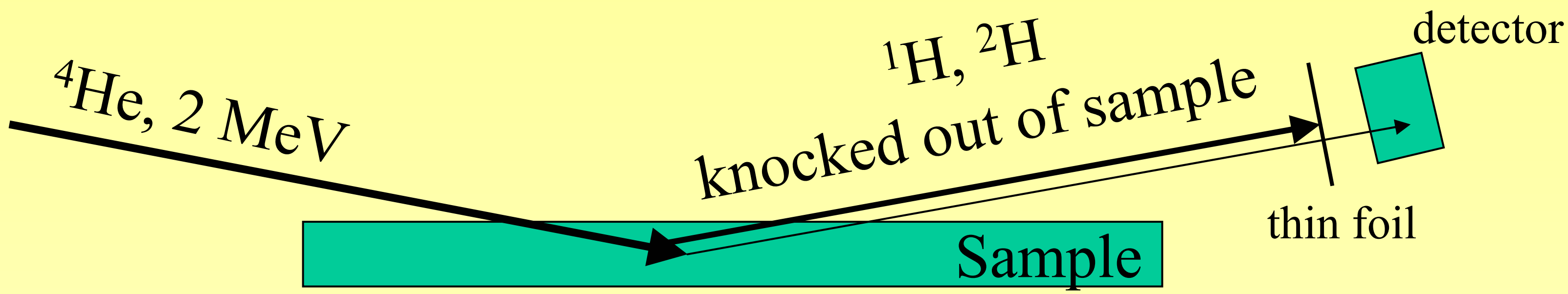
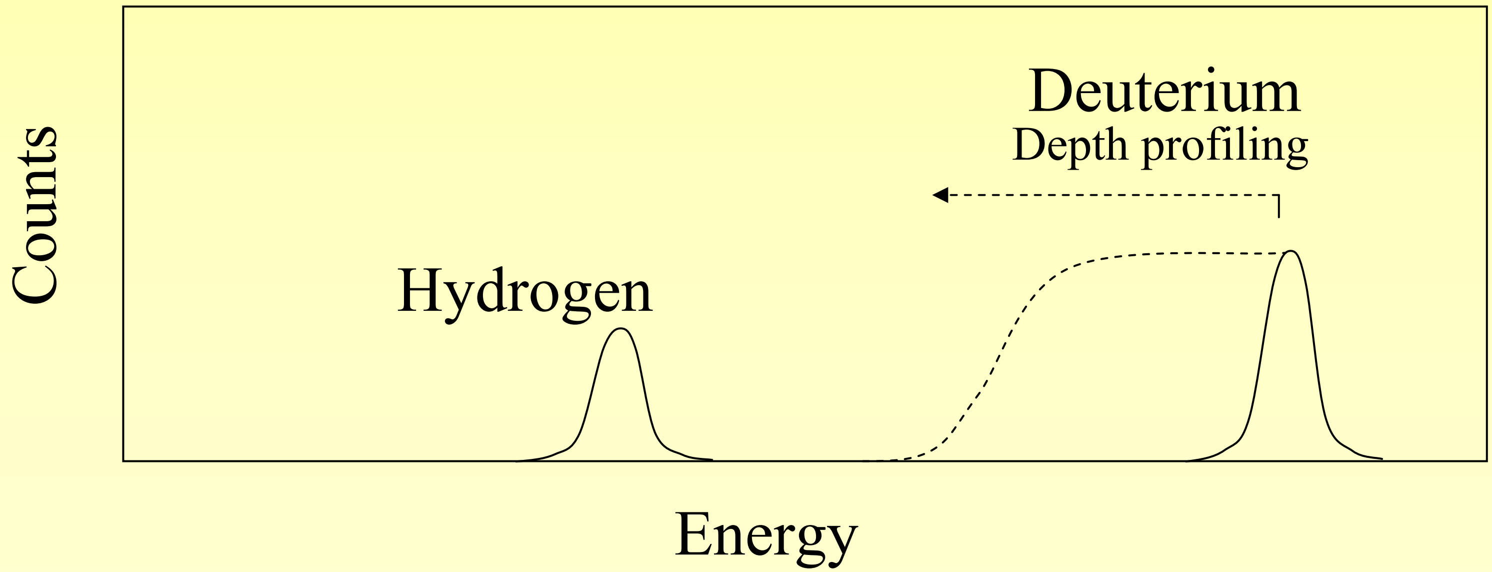
# What we have not talked about

## Elastic Recoil Detection



# Concluding observations

Stopping powers are essential. They are largely under control with SRIM2003, but in specific cases can be up to 10% in error.

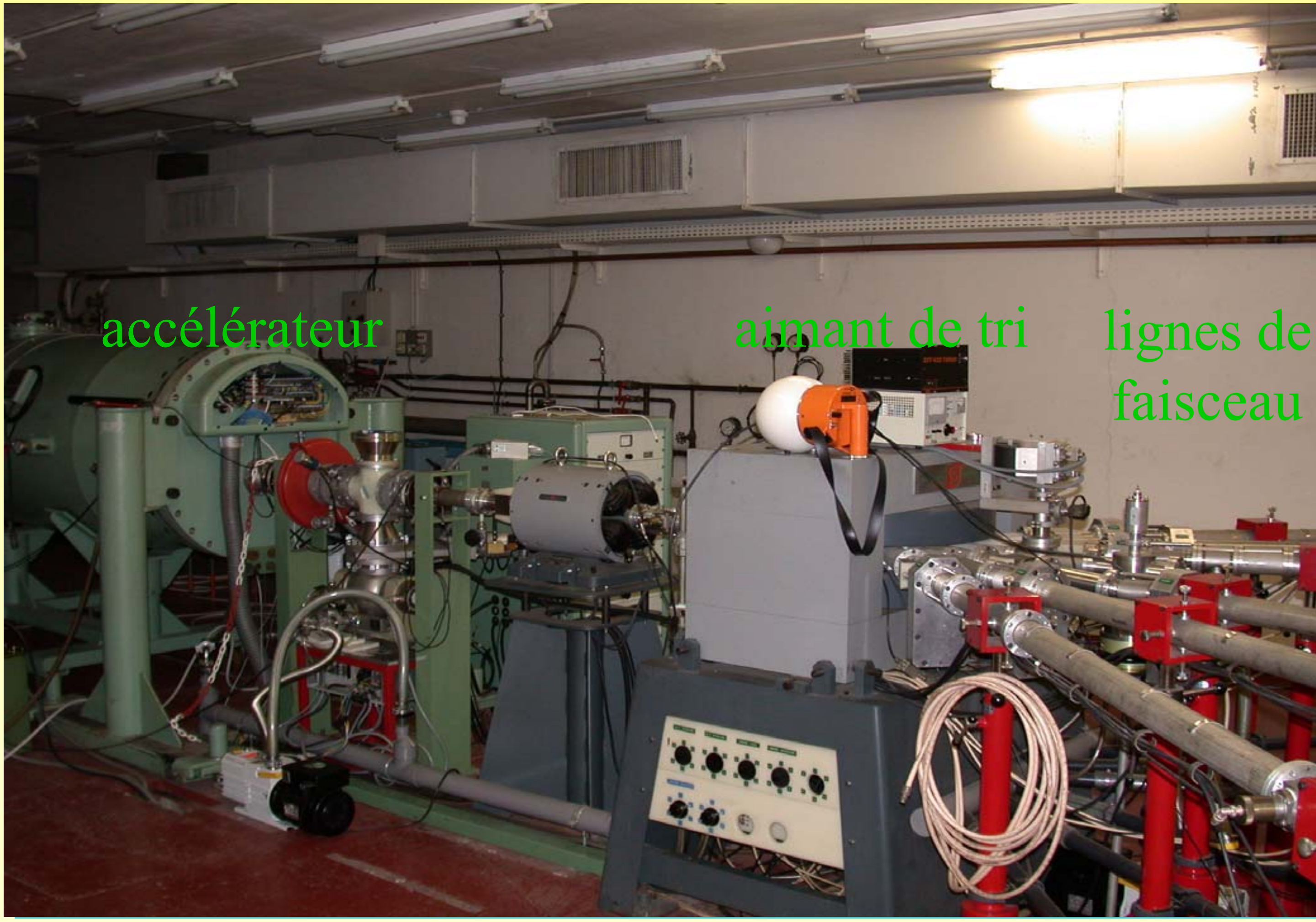
Many nuclear reaction and non-Rutherford elastic scattering cross sections are available from SigmaBase, NRABase and SimNra. A partially fragmented 'Cottage Industry' in need of central coordination. Evaluation is under way (Gurbich/SigmaCalc)

(cp,γ) spectra and thick target yields from literature

- Efforts are under way to include cp cross-sections for IBA in Exfor, and provide for extraction of data in appropriate computational format

# Système d'Analyse par Faisceau d'Ions Rapides

## Production de faisceau




Accélérateur
1 turbo

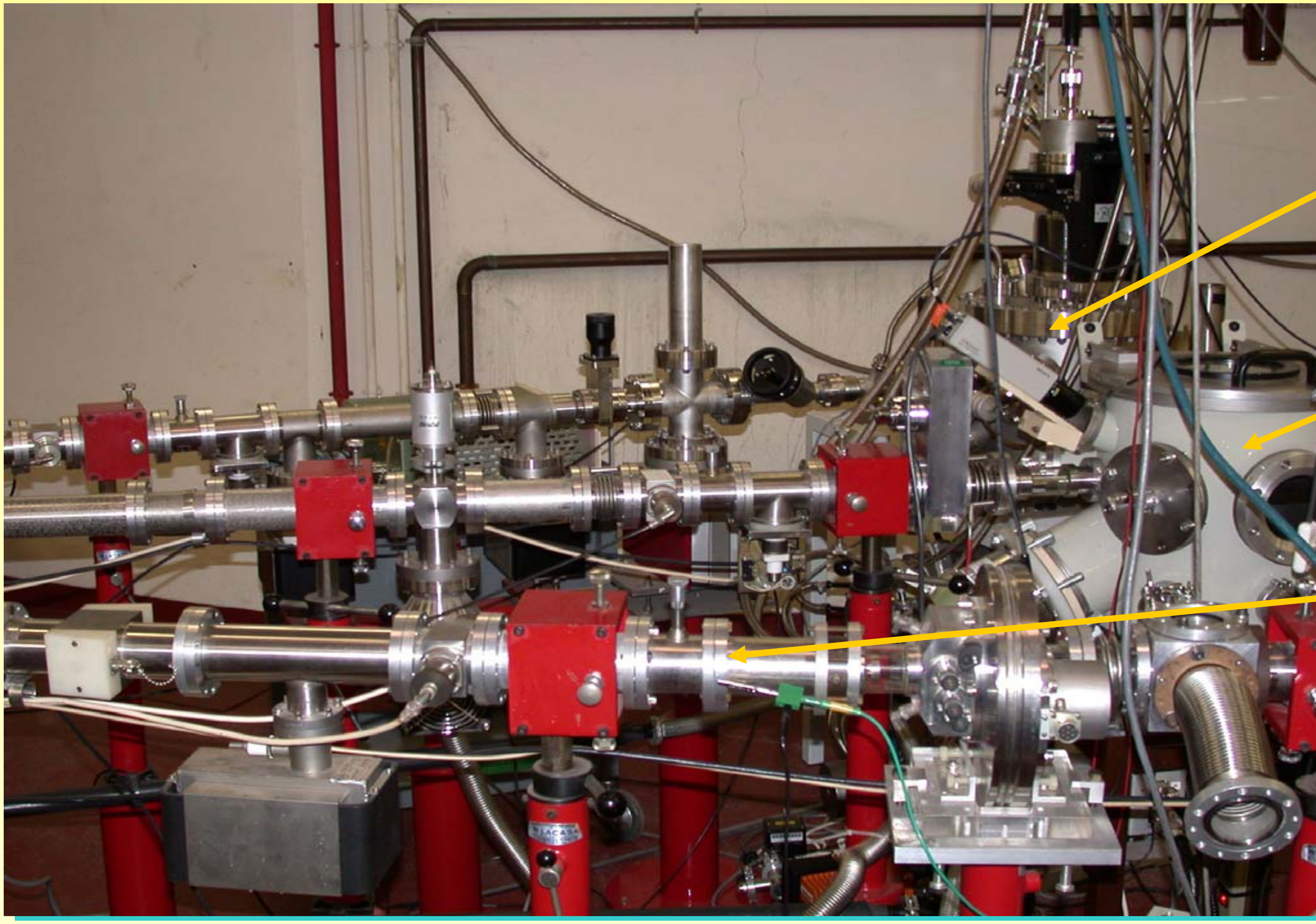
Aimant
1 turbo

# Lignes et chambres d'expériences

## Lignes gauches

Chaque ligne
1 turbo

Chaque chambre
1 turbo



Chambre 'in-situ'

Pompage différentiel

Pompes ioniques

Chambre polyvalente

Ligne pour MEIS

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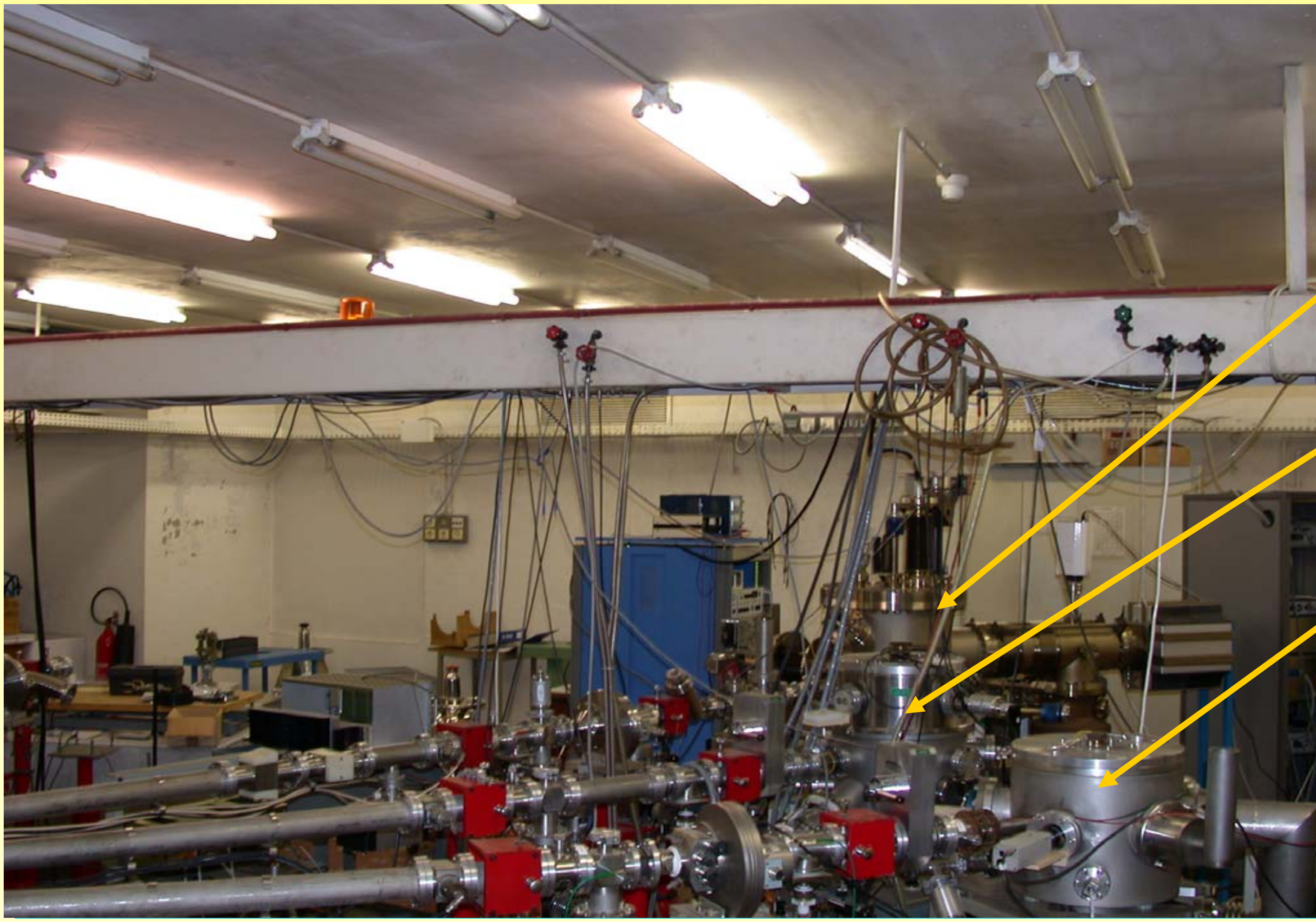
# Lignes et chambres d'expériences

## Lignes droites

Chaque ligne
1 turbo

Chaque chambre
1 turbo



Chambre UHV/surfaces

Pompage différentiel
Pompes ionique, à sublimation

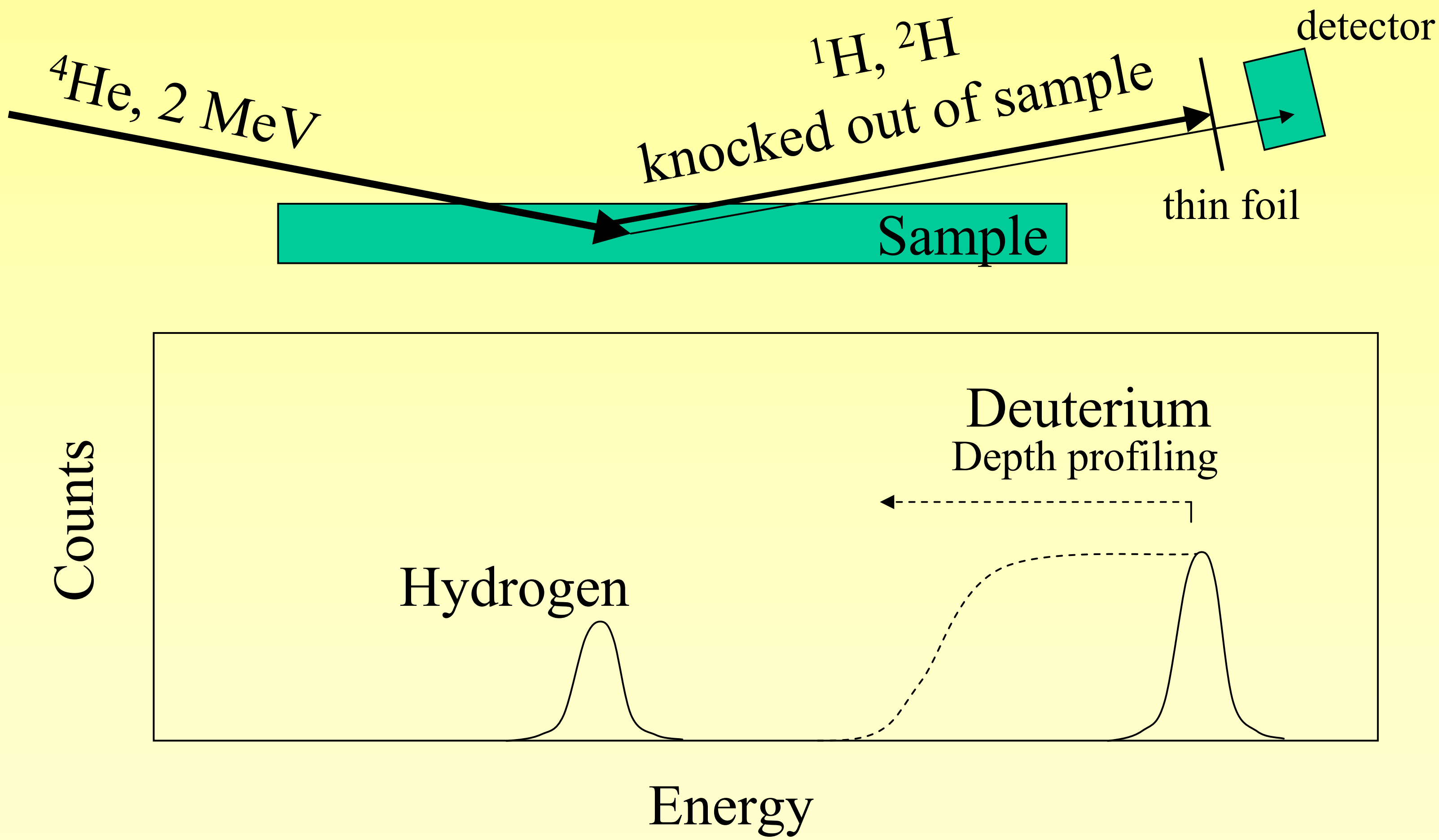
Chambre canalisation

Chambre polyvalente/ERD

# End of Overview

# Coffee !

# ERD - Principle

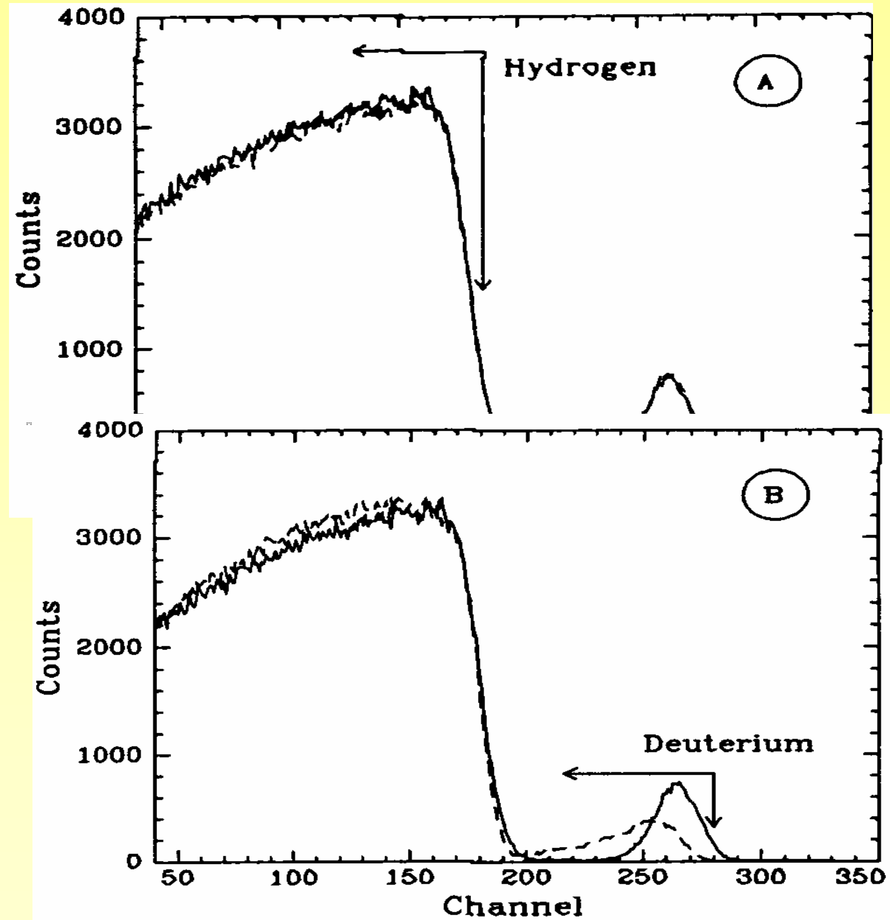


# ERD - Characteristics

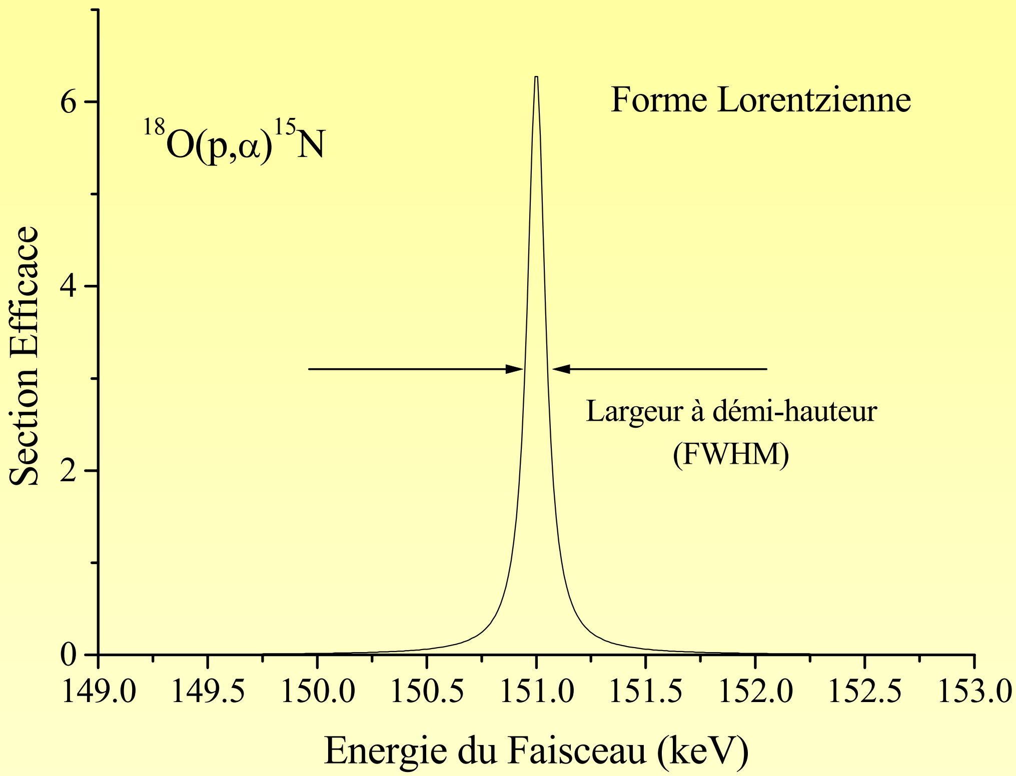
- Depth resolution, a few $10^2$ Å
- Sensitivity - similar to RBS
- Explorable depth, 1 - 2 µm
- Isotopic sensitivity ($^{1}H/^{2}H$)

# ERD Example

Diffusion of a dueterium-labelled polystyrene layer into unlabelled polystyrene

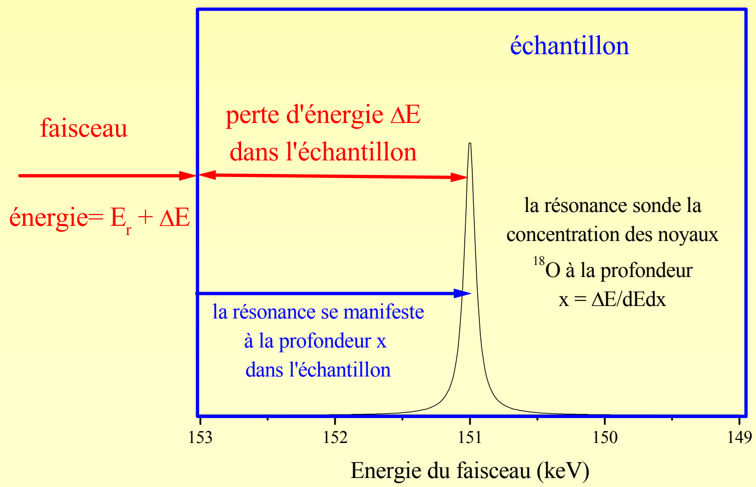


# A narrow nuclear resonance



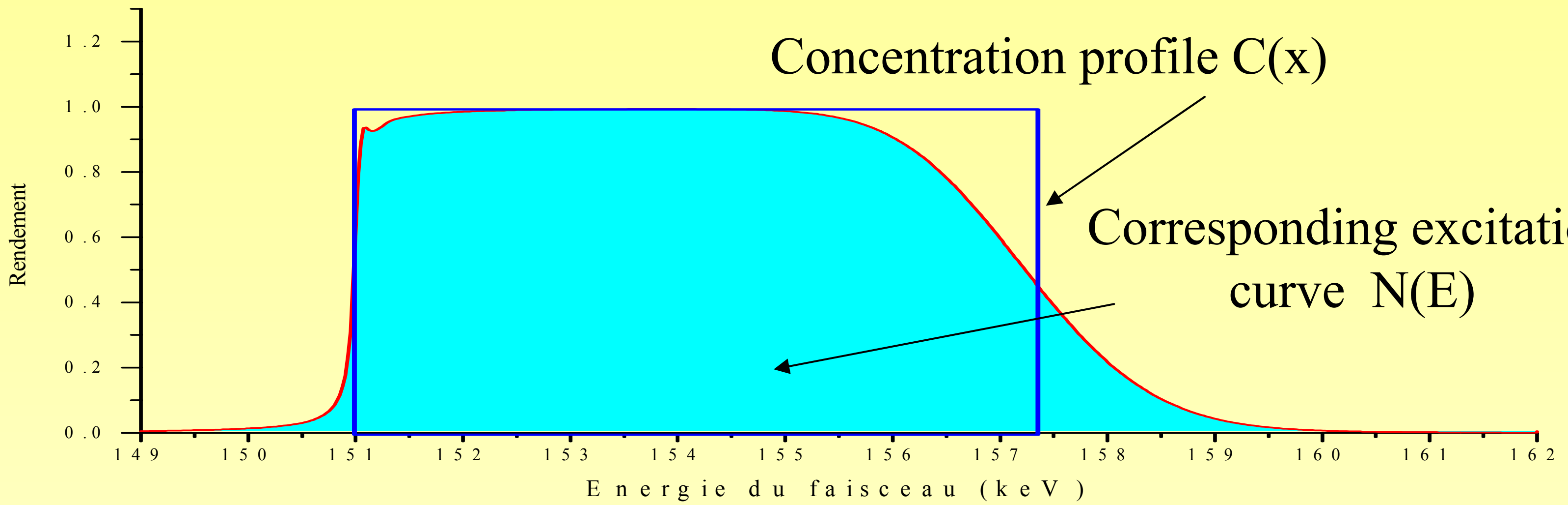
# Determining Concentration Profiles

- The resonance is scanned through the target depth by scanning the incident beam energy



# An excitation curve

$^{18}O(p,\alpha)$ 151 keV $\Gamma$=100 eV



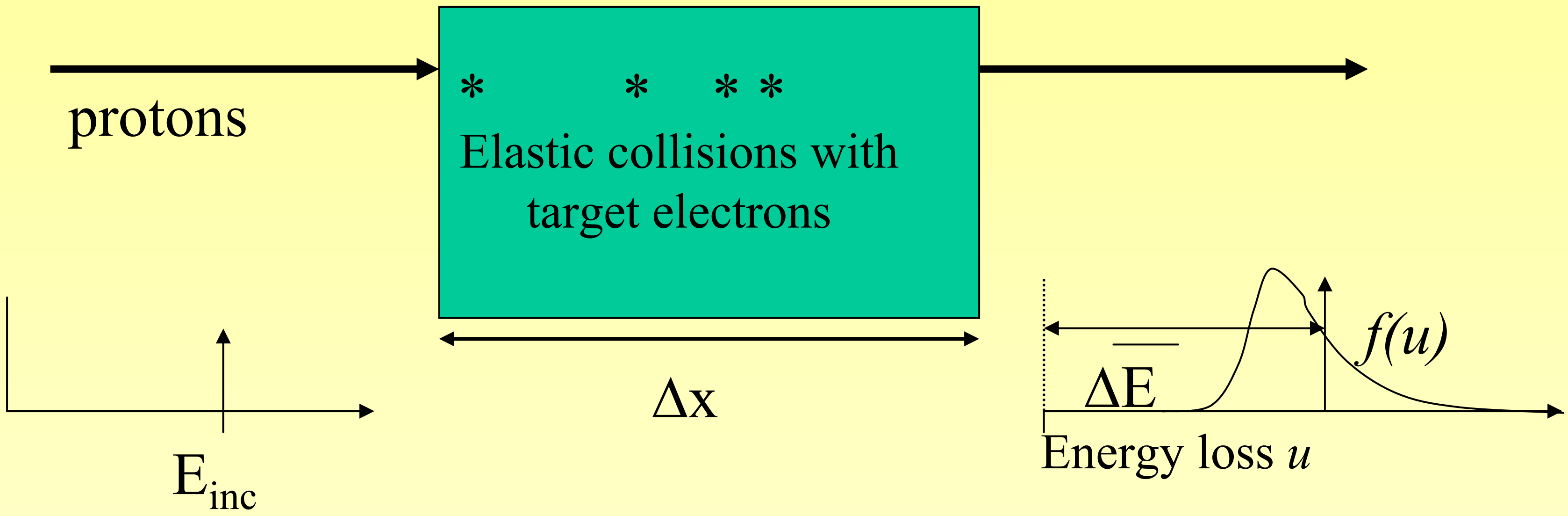

$$N(E) = G(E) * W(E) * T(E) * S\langle C(x) \rangle$$

$$S\langle C(x) \rangle = \sum_{n=0}^{n=\infty} k_n f^{*n}(u)$$

$G(E)$ beam + Doppler energy spread
$W(E)$ rersonance lineshape
$T(E)$ beam energy straggling
S<C(x)> ‘ straggling ’ of C(x)

# Charged particle energy loss

The charged particles lose their energy in independant collisions with electrons

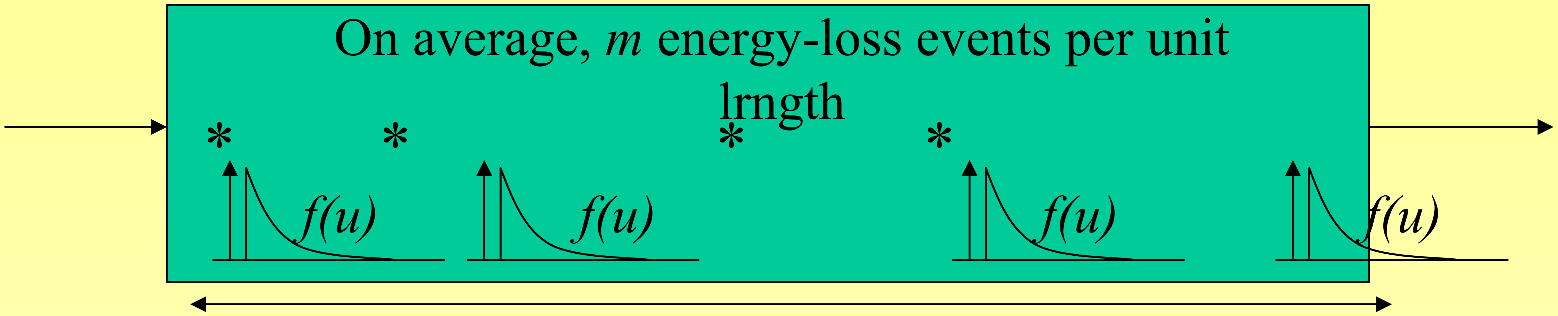



The stopping power dEdx $\equiv \lim_{\Delta x \to 0} \frac{\Delta E}{\Delta x}$

The straggling constant S is defined by

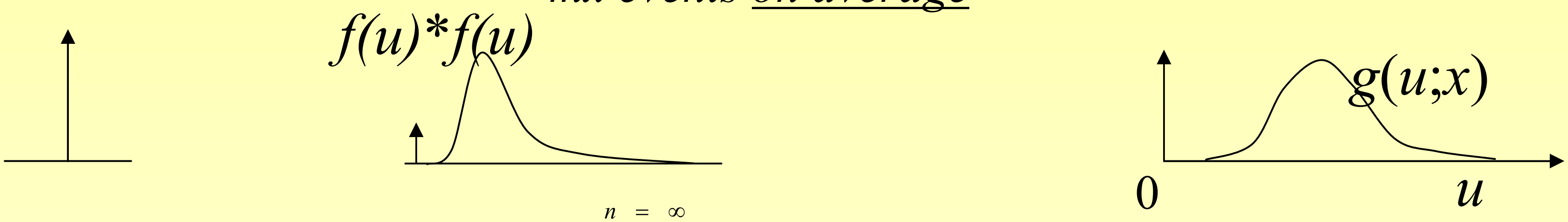
$$\sigma\left(f(u)\right) \equiv S\sqrt{\frac{2Z}{A}}\sqrt{x}$$

# Straggling




*For thickness x*

*mx events* *<u>on average</u>*



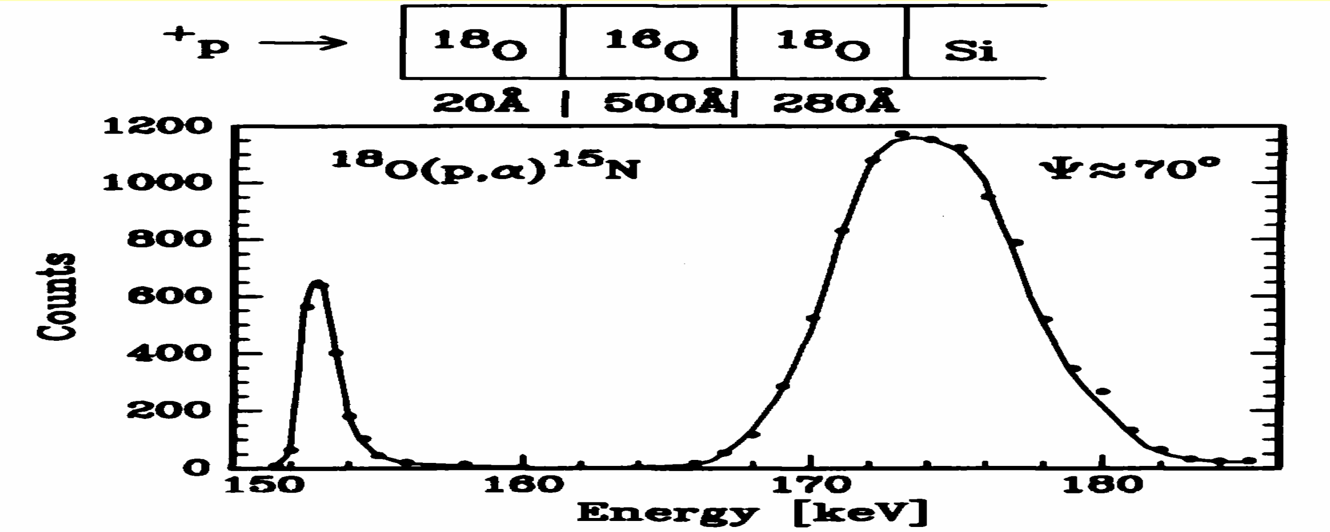

$$g(u;x) = \sum_{n=0}^{n=\infty} P_n(mx)\, f^{*n}(u)$$

$$P_n(mx) = e^{-mx}\frac{(mx)^n}{n!}$$

- g(u;x) tends towards a Gaussian for large x

# Narrow resonance profiling - example

Sequential oxidation of silicon in $^{16}O$, then $^{18}O$



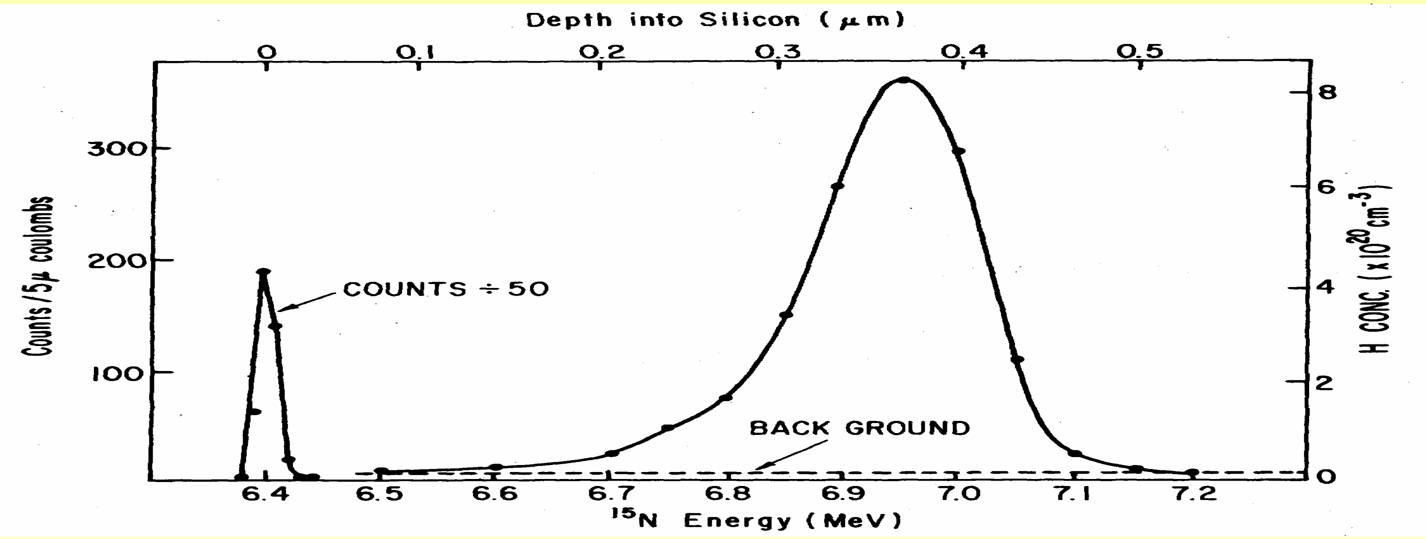

*From G. Battistig et al, NIMB66 (1992) 1-10*

# Hydrogen profiling with a nuclear resonance

Hydrogen implantation profile in silicon ($10^{16}$ $cm^{-2}$, 40 keV)

*from W.A. Lanford, NIMB66(1992),68*

$^{1}H(^{15}N,\alpha\gamma)^{12}C$




*from W.A. Lanford, NIMB66(1992),68*

# IBA methods

– **PIXE**
  - **P**article-**I**nduced **X**-ray Emission

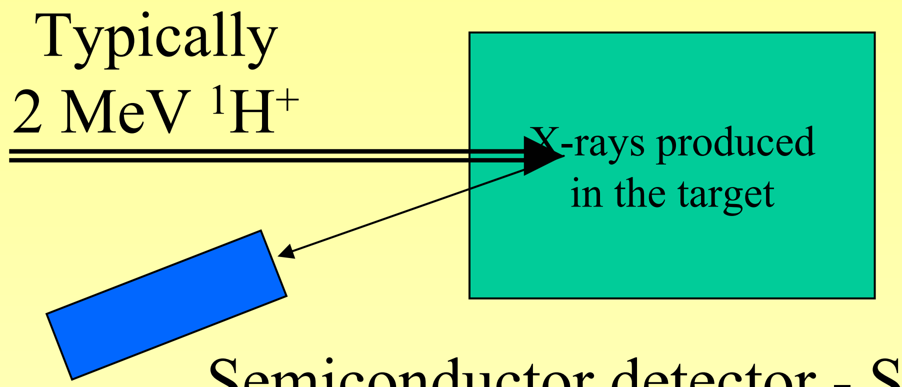
– **ERD or FRS**
  - **E**lastic **R**ecoil **D**etection **A**nalysis or
  - **F**orward **R**ecoil **S**pectrometry

$$\frac{d\sigma}{d\Omega}$$

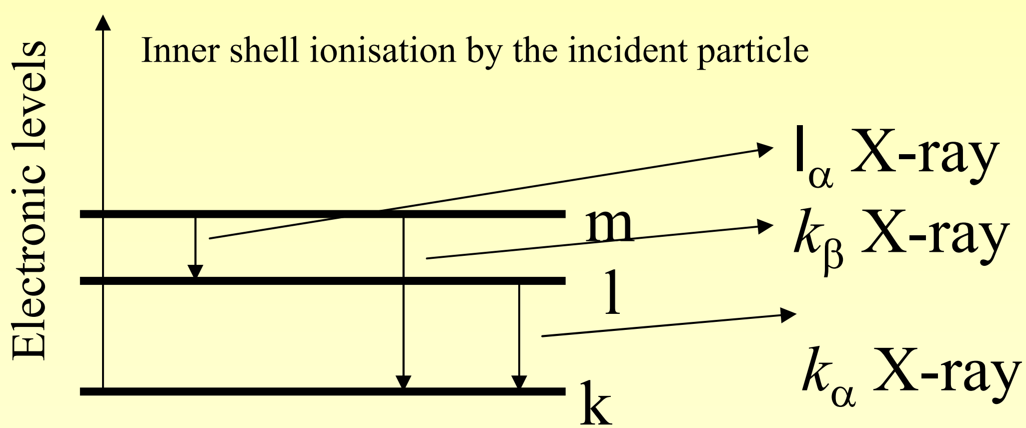
– **RBS-Channeling**
  - **R**utherford **B**ackscattering **S**pectrometry

– **NRA (NRP, PIGE)**
  - **N**uclear **R**eaction **A**nalysis
  - **N**uclear **R**esonance **P**rofiling
  - **P**article-**I**nduced **G**amma **E**mission

# PIXE - Principle

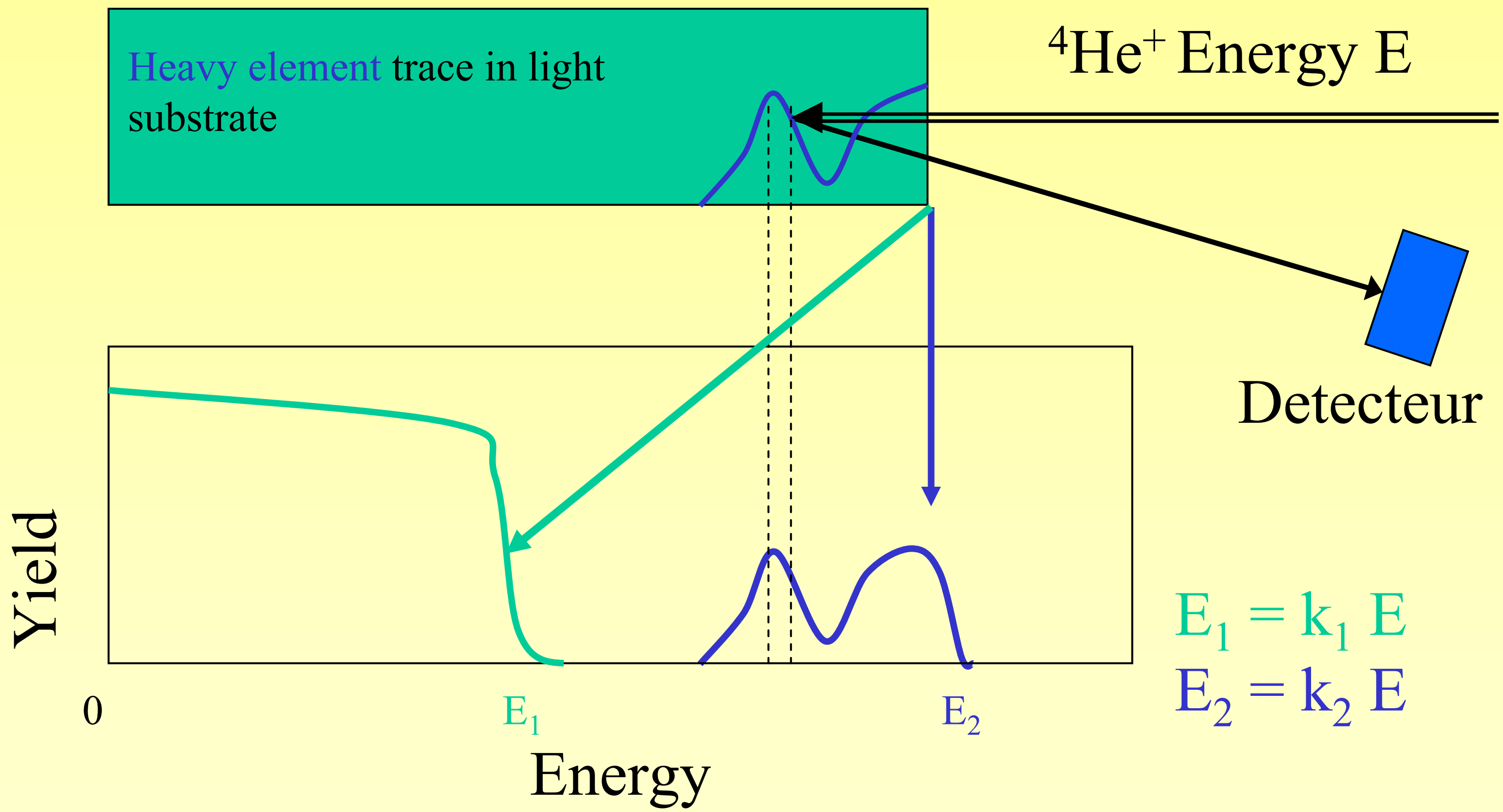



Semiconductor detector - Si(Li), Peltier-cooled

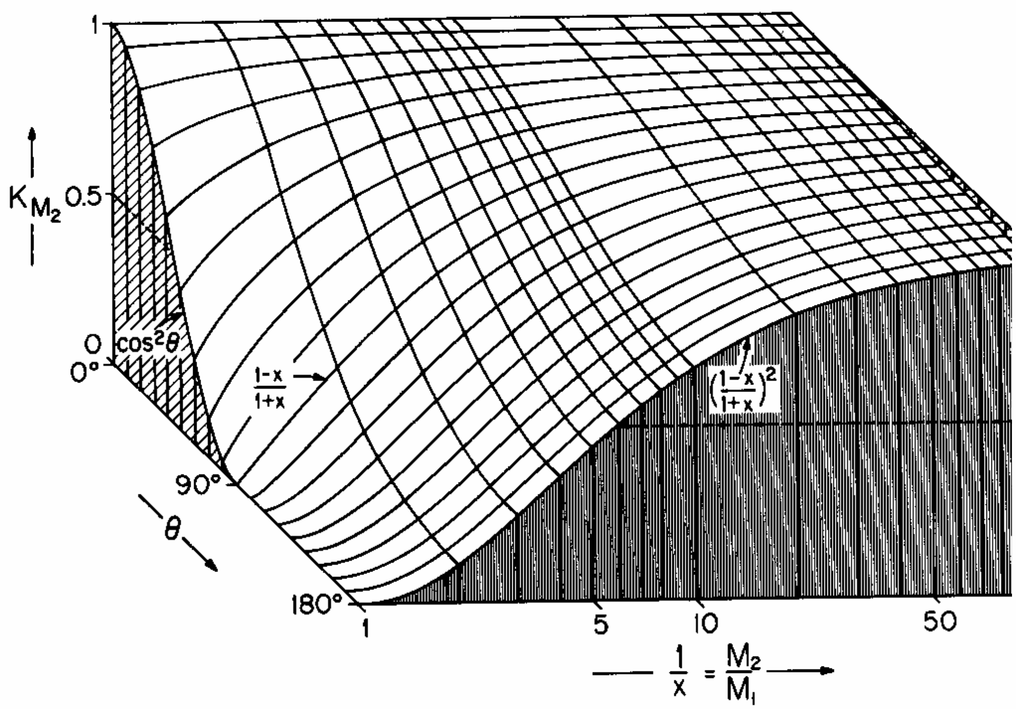


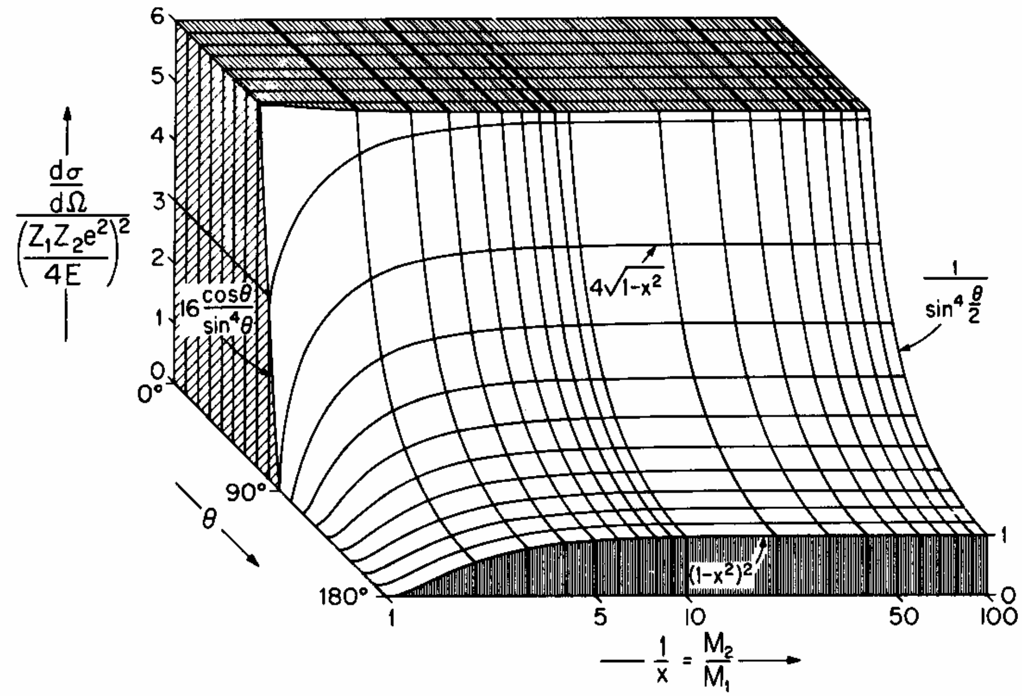

Characteristic X-ray emission
-> element identification

# RBS - principle



# RBS - détails



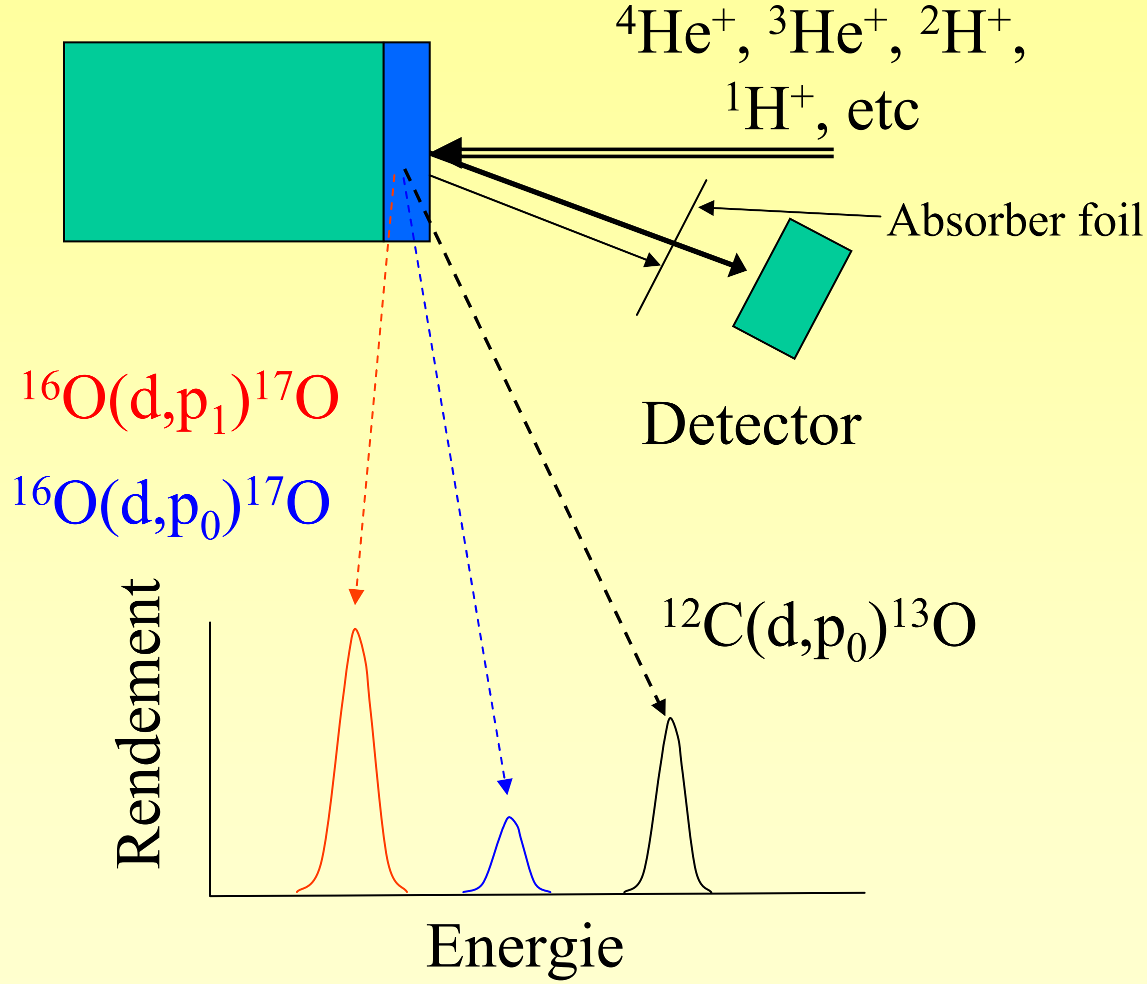



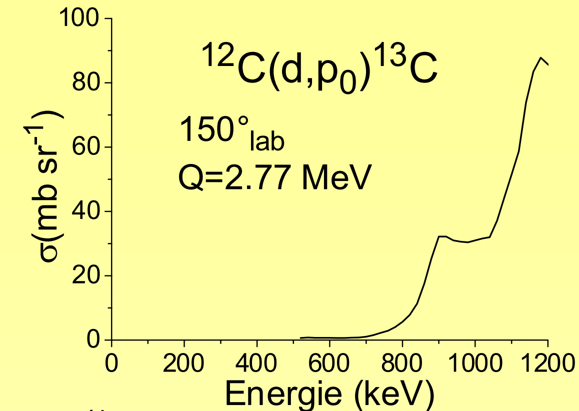

Kinetics

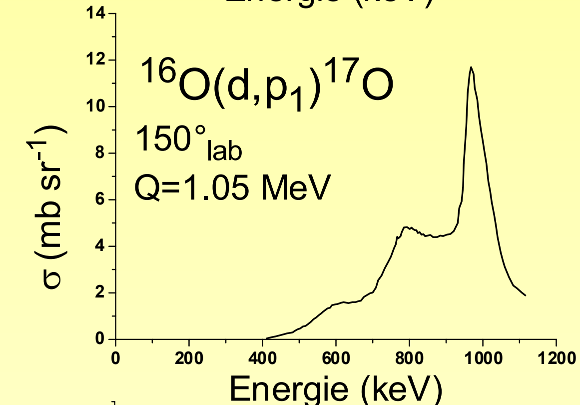
Section efficace de Rutherford

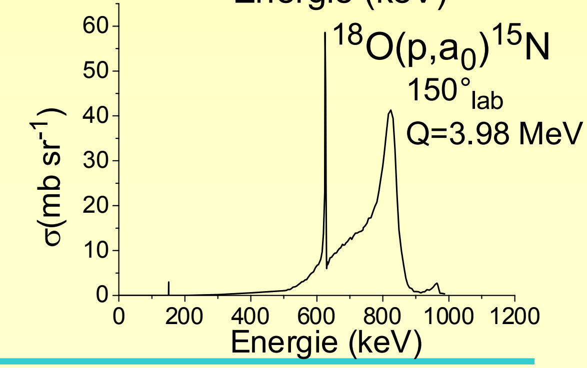
piqué dans 'Backscattering Spectrometry', Chu, Mayer and Nicolet, Academic Press, 1978

# NRA - principle

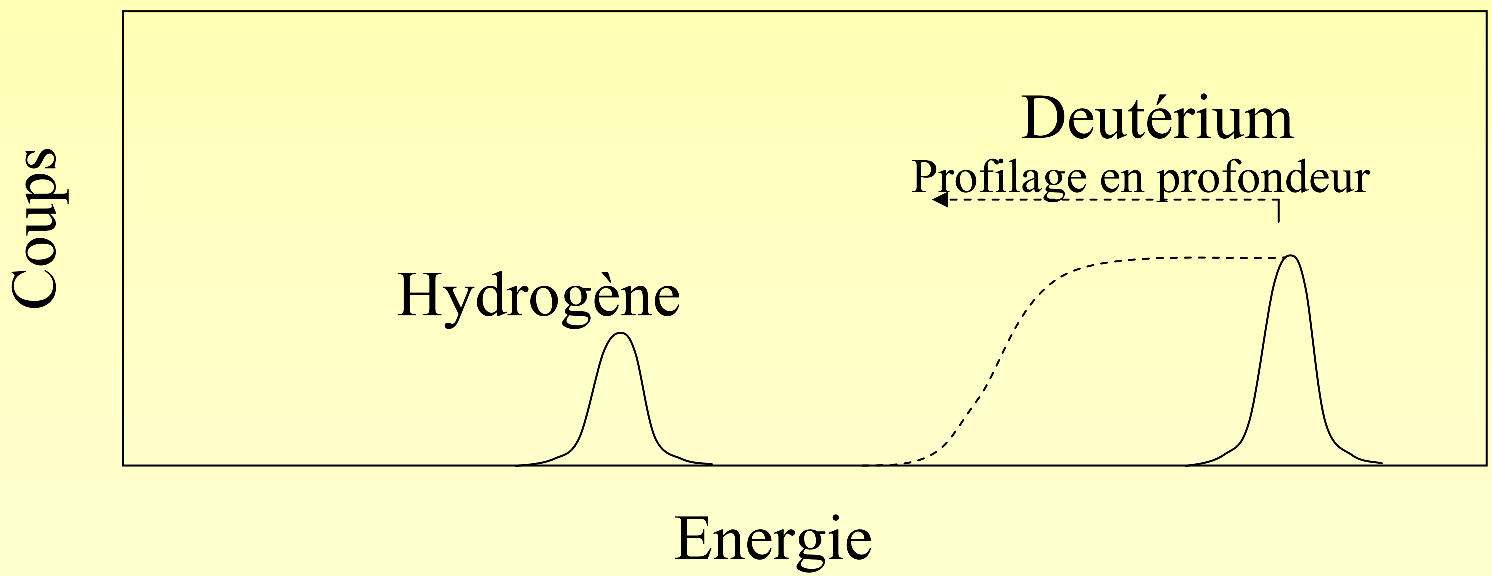


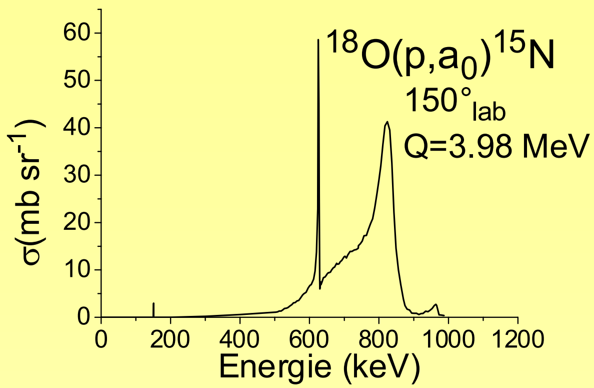



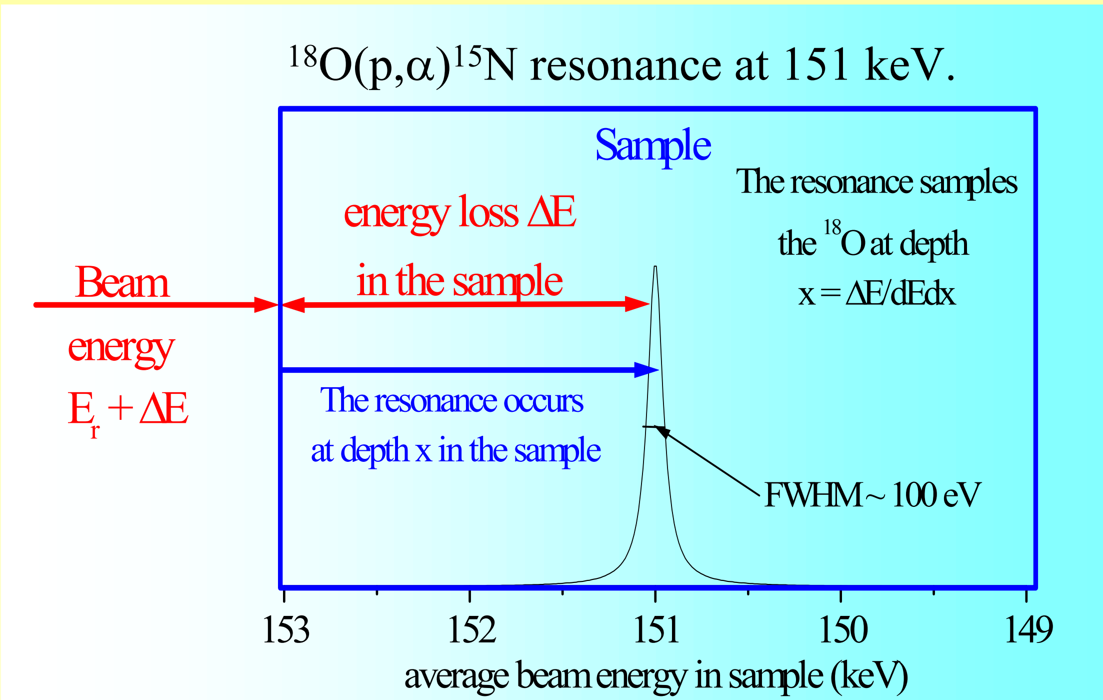



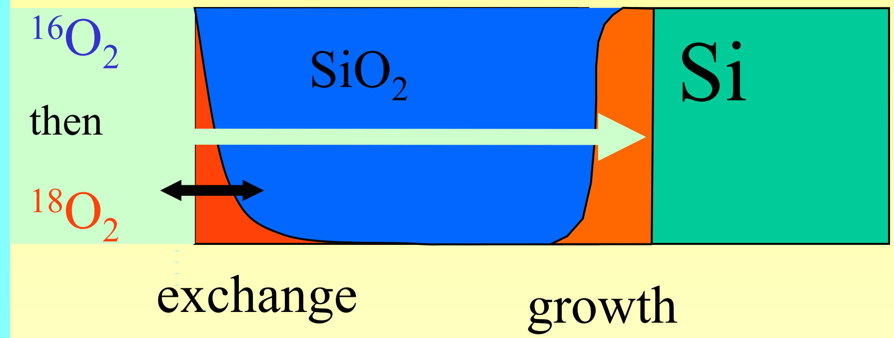
# ERD - Principe

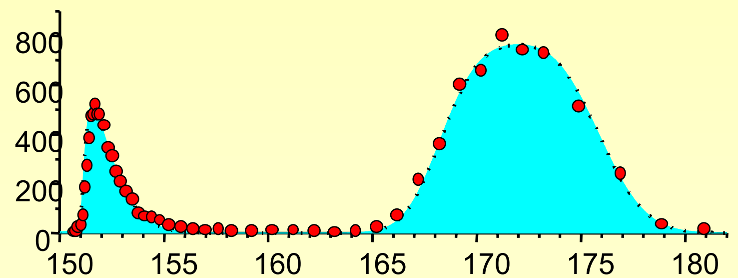






# Profilage par résonance étroite nucléaire et traçage isotopique

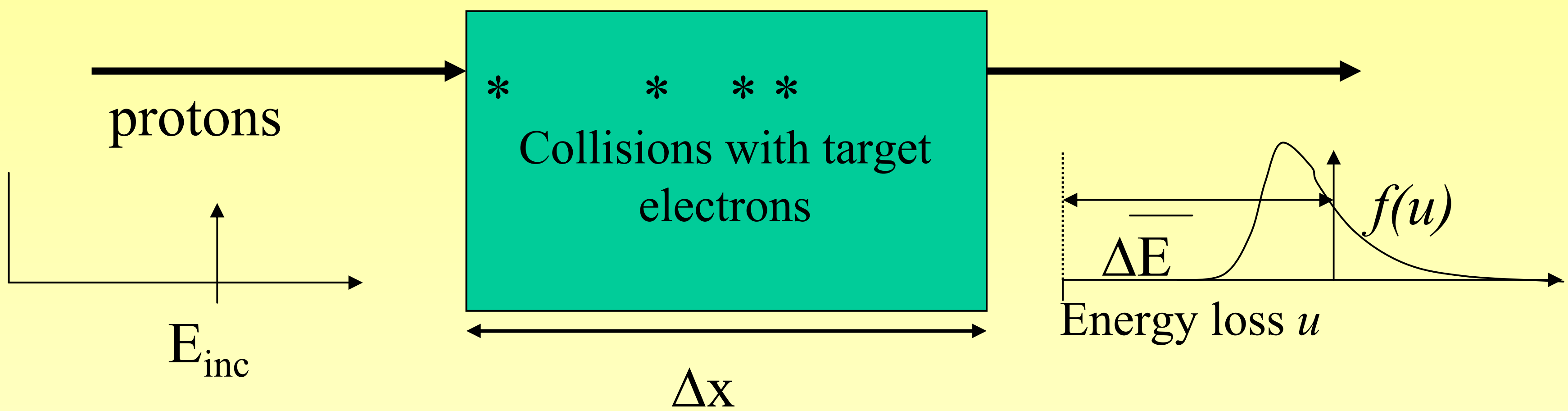


# Charged particle energy loss

The charged particles lose their energy in independant collisions with electrons

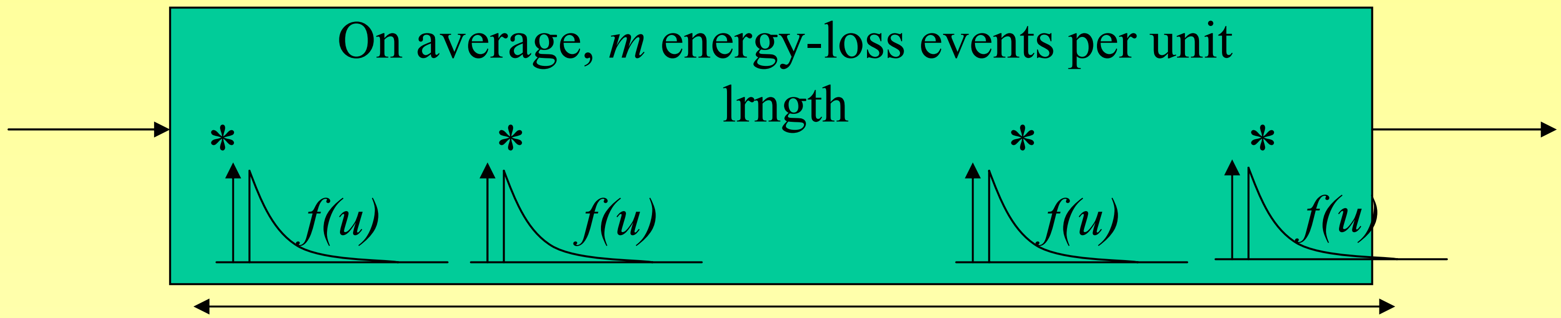



The stopping power dE/dx $\equiv \lim_{\Delta x \to 0} \dfrac{\Delta E}{\Delta x}$

The straggling constant S is defined by

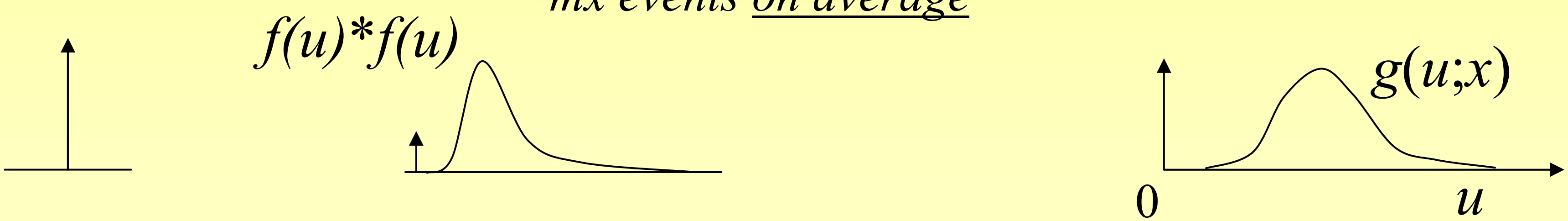
$$\sigma\left(f(u)\right) \equiv S\sqrt{\frac{2Z}{A}}\sqrt{x}$$

# Straggling




*For thickness x*

*mx events on average*




$$g(u;x) = \sum_{n=0}^{n=\infty} P_n(mx) f^{*n}(u)$$

$$P_n(mx) = e^{-mx} \frac{(mx)^n}{n!}$$

- g(u;x) tends towards a Gaussian for large x