Quantitative considerations in medium energy ion scattering

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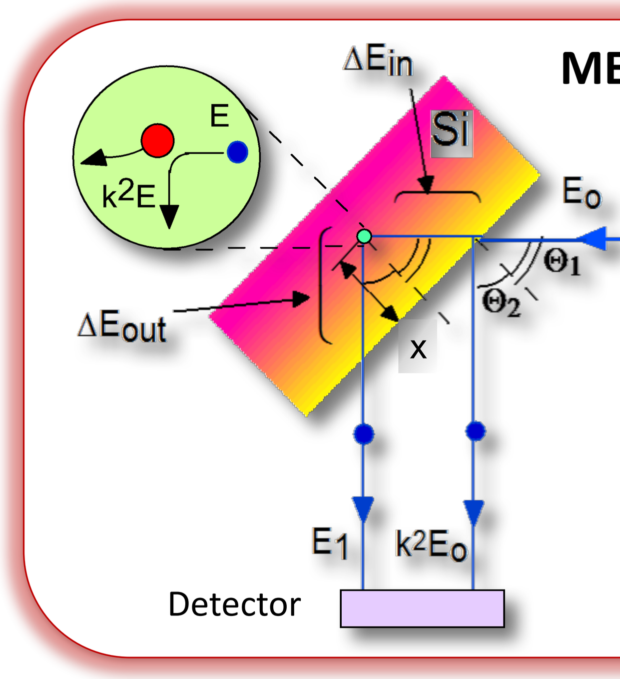
Introduction

Due to its unique capability of providing **near-quantitative compositional and layer structure information during depth profiling analysis,** in favourable cases, with sub-nanometre resolution, medium energy ion scattering (MEIS) is becoming increasingly important to the characterisation of microelectronic device structures in which scaling laws have driven the growth and doping of layers of nanometre thickness. **Here we assess the quantitative accuracy in terms of both depth and concentration, that can be achieved in MEIS depth profiling.**

MEIS basics

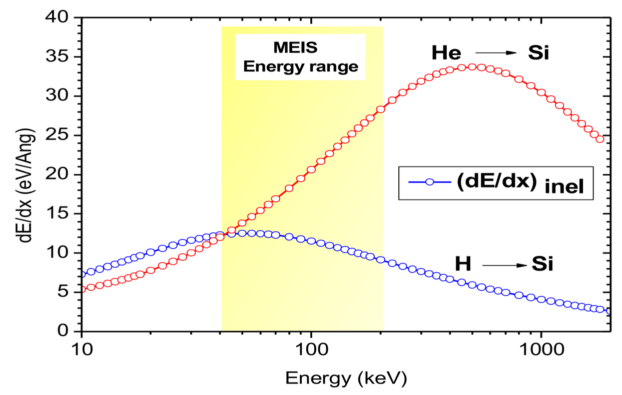


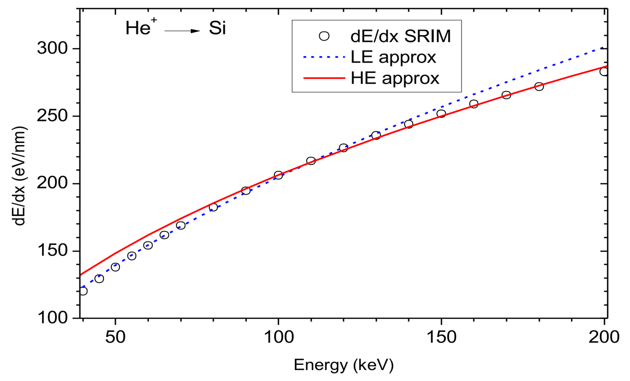
- **Elastic energy loss** yields the **mass** of the atom scattered off
- **Inelastic energy loss** within the sample enables **depth analysis**

Backscattering of 50 - 200 keV H⁺ or He⁺ ions off shallow implants, nanometre thin overlayers and thin films on top of a Si (100) surface.

Inelastic energy loss to depth scale conversion

Depth scales in MEIS are derived from the inelastic energy loss of the scattered projectiles on the way in and out.





The **energy loss rate dE/dx** is dependent on the energy of the projectile and can be obtained from SRIM calculations, shown for for H^+ & He^+.

For the energies used in MEIS the electronic loss rates can be well approximated by a power law:

$$-\frac{dE}{dx} = AE^B \qquad (1)$$

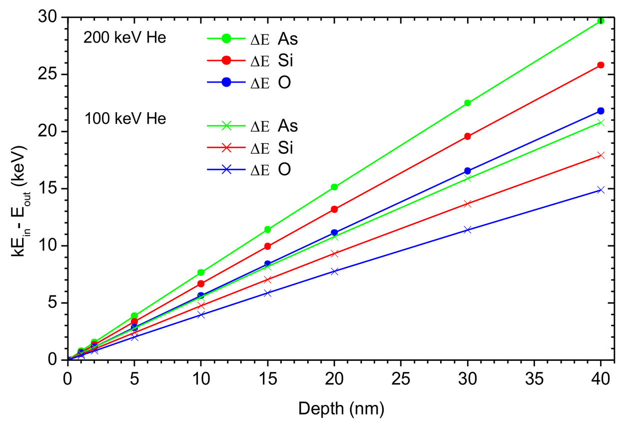
e.g. low E approx. (40-100 keV)
A= 0.043, B = 0.58 (1%)

or: high E approx. (80-200 keV)
A= 0.0248, B= 0.46 (1%)

NB. *dE/dx* in keV/nm, *E* in keV.

Eq.(1) enables **a fully analytical conversion of inelastic energy loss to pathlength:**

$$pathlength = \int_{E_{start}}^{E_{finish}} \frac{1}{-dE/dx}\, dE = \frac{1}{(1-B)A}\left[E_{start}^{1-B} - E_{finish}^{1-B}\right] \qquad (2)$$



Example: 100 & 200 keV He^+ ions incident on a ^{28}Si (100) surface, containing O and As; Θ = 90°; Θ_1 = 35.26° & Θ_2= 54.74°.

Apply **i)** eq.(2) on the way in, then **ii)** the **kinematic factor *K*** (Θ = 90°)

$$K=(M_{target}-M_{ion})/(M_{target}+M_{ion})$$

and finally **iii)** eq. (2) on the way out, This gives $kE_{in}-E_{out}$ vs **depth** to 40nm (using a Si density of 5 x 10^{22} at/cm³)

NB.
- The **near-linear** relationship between KE_{in}-E_{out} & **depth** (for depths ≤40 nm)
- Substantial differences between slopes for Si , As and O by up to 15%

Approach is also valid for compounds. For multilayered samples, A will be different for each layer but B changes little; but now computer simulations are required.

Peakheights ratios

The absolute backscattering yield of target atoms at a depth x in a homogeneous target is according to Chu et al. (Backscattering Spectrometry, 1978)

$$H(E_{out}) = \sigma(E)\;\Omega\;\Phi\;\frac{D}{[\varepsilon(E)]\cos\theta_{in}}\;\frac{\varepsilon(KE)}{\varepsilon(E_{out})} \qquad (3)$$

where E_{out} is the energy at the detector after scattering off a target atom at depth *x*, *E* is the energy immediately before scattering at that depth, σ(*E*) the energy-dependent Rutherford scattering cross section, Ω the detector acceptance angle, Φ the total number of incident particles, *D* the detector energy bin or channel width, ε the stopping cross section, and *K* the kinematic factor for the scattering geometry adopted.
[ε(E)] is called the stopping cross-section factor (Chu et al.):

$$[\varepsilon(E)] = \frac{K}{\cos\theta_{in}}\frac{1}{N}\frac{dE}{dx}\Big|_E + \frac{1}{\cos\theta_{out}}\frac{1}{N}\frac{dE}{dx}\Big|_{KE} \qquad (4)$$

The term *D* is given as:

$$D = [\varepsilon(E)]N\tau \qquad (5)$$

N is the atom density and τ the thickness of the surface layer across which an ion will lose the energy equivalent to the width of a single bin within the detection system.

For scattering at the top surface $E = E_0$ and $E_{out} = KE_0$ so that the final term in eq. (3) disappears; the yield off the surface is then:

$$H(KE_0) = \sigma(E_0)\;\Omega\;\Phi\;\frac{D}{[\varepsilon(E_0)]\cos\theta_{in}} \qquad (6)$$

The change in yield due to scattering off atoms at depth *x* as a ratio to scattering off atoms at the surface follows directly as:

$$\frac{H(E_{out})}{(H(KE_0))} = \frac{\sigma(E)}{\sigma(E_0)}\cdot\frac{[\varepsilon(E_0)]}{[\varepsilon(E)]}\cdot\frac{\varepsilon(KE)}{\varepsilon(E_{out})} \qquad (7)$$

as long as the detector channel width D is independent of energy (as in RBS - surface barrier detectors). Factors like Ω, Φ and cosθ_{in} have cancelled in eq. (7). The Rutherford cross section is σ ∝ E^{-2}. The scattering geometry dependent stopping cross section factors [ε], are defined in eq. (4); again constants such as the atomic density are ignored in this analysis which is permissible since only ratios of either ε's or [ε]'s are considered here. The benefit of the power law eq.(1) is now clear since:

$$\frac{[\varepsilon(E_0)]}{[\varepsilon(E)]} = \left(\frac{E_0}{E}\right)^B \quad \text{and} \quad \frac{\varepsilon(KE)}{\varepsilon(E_{out})} = \left(\frac{KE}{E_{out}}\right)^B$$

so that eq. (7) reduces to:

$$\frac{H(E_{out})}{H(KE_0)} = \left(\frac{E_0}{E}\right)^2\cdot\left(\frac{KE_0}{E_{out}}\right)^B \qquad (8)$$

I.e. deviations from the energy dependence of the yield according to the Rutherford prediction (1st term eq. (8)) **scale with the inverse ratio of the energies *at the detector* (E_{out}) to a power *B* ≈ ½** (2nd term eq. (8)). B depends mainly on energy, little on material type. Acquisition software makes D independent of E in our MEIS instrument.

Using eq.2 for the previous example we get: **H(x)/H(0) = 1 + 0.0055x i.e < 1% /nm**
Slope varies with geometry but is almost independent of atom type.

Screening correction

In the MEIS energy regime the nuclei are partially screened during the interaction. The Rutherford scattering cross section is not exactly valid and need a correction. Following Andersen [Phys Rev A21 (1980)1891] for a screened Coulomb potential:

$$V(r) = \frac{Z_i Z_t e^2}{r}\,\varphi\!\left(\frac{r}{a}\right) \qquad (9)$$

Z_i and Z_t are the atomic numbers, φ (*r*/*a*) is the so-called screening function and *a is* the screening length, that depends on Z_i and Z_t . At *r* =0, φ =1 (Coulomb pot.). Expanding φ near *r* =0 to first order in a Taylor series yields:

$$\varphi\!\left(\frac{r}{a}\right) \approx 1 + \frac{r}{a}\,\dot{\varphi}(0) \qquad (10)$$

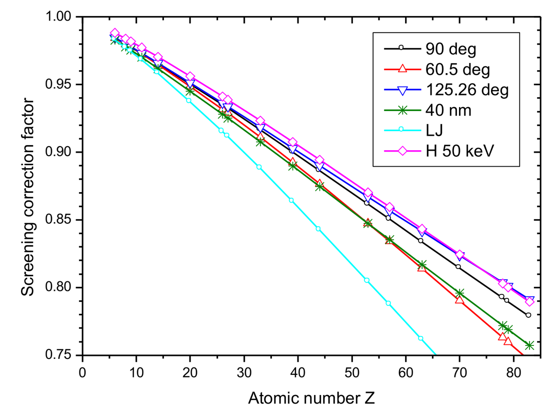
with $\dot{\varphi}(0)$ the gradient of the screening function *r* = 0. Inserting eq. (10) into eq. (9) gives:

$$V(r) = \frac{Z_i Z_t e^2}{r} + \frac{Z_i Z_t e^2}{a} = V_{coulomb} + V_{const} \qquad (11)$$

$\dot{\varphi}(0)$ is negative; **screening *decreases* the Coulomb potential** by a constant amount. Andersen et al. incorporated this by ***increasing* the kinetic energy** of the projectile in the CoM system by exactly the same amount.

E is now replaced by $E+V_{const}$ in the Rutherford cross section. The net effect is to decrease the scattering cross section progressively with increasing Z_t.
In the CoM system the **screening correction factor P_{scr}** can now written as:

$$P_{scr} \equiv \frac{\sigma(E_0+V_{const})}{\sigma(E_0)} = \left(1+\frac{V_{const}}{E_0}\right)^{-2} \approx 1 - f\,\frac{Z_i Z_t}{E_0} \qquad (12)$$



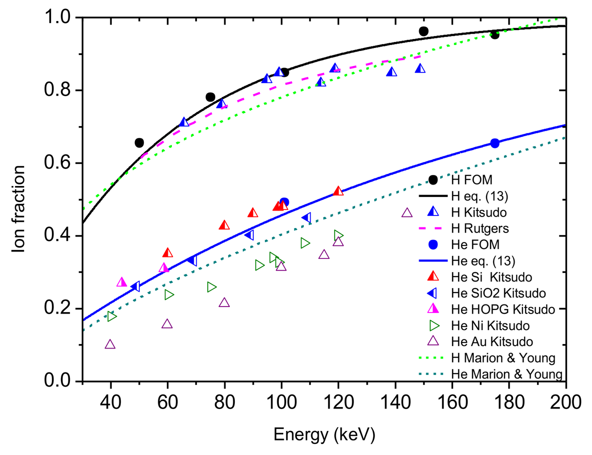
Example:
- 100 keV He^+ ions scattered off surface C to Bi (Z_t= 6-83) @ 60.5°, 90° and 125.26°.
- 100 keV He^+ ions @ 90° off depth 40 nm
- 50 keV H^+ ions @ 90°

using the Biersack-Ziegler universal potential (5x) and Lens-Jensen (L J) 1x.

NB:
- P_{scr} depend almost linearly on Z_t
- P_{scr} is similar for Z_t/E_0 = constant (cf. **50 keV H⁺** similar to **100 keV He⁺**).
- *f* is almost constant and depends mainly on choice of potential (e.g. L J)
- *f* depends weakly on scattering angle and depth.
- *f* = 0.16 ± 0.04 (max intrinsic error)

Neutralisation correction

In MEIS the velocities of the H^+ or He^+ ions are moderate and a fraction of the scattered projectiles leave the surface neutralised. When using electrostatic analysers (unlike for TOF ones) these particles are not counted, but cannot be ignored in quantitative analysis. Fractions of particles leaving ionised are not generally accurately known. Shown below are data measured by various groups for H and He projectiles as as a function of energy.

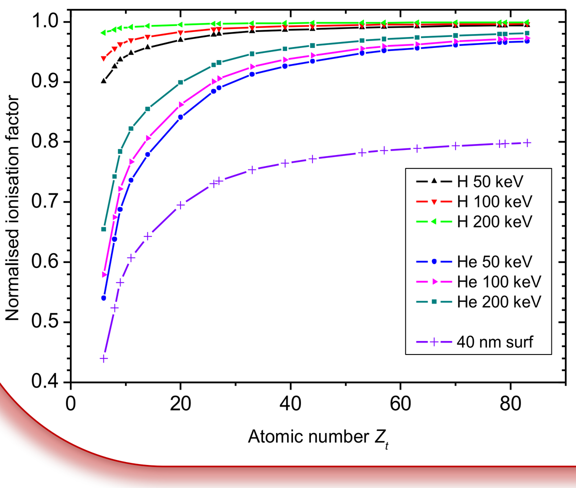


FOM group data library of 50 sets at 5 different energies (collated by Bailey) (no clear dependence on target atom)

Kido group (Kitsudo et al. NIMB **267**, (2009) 566) (some dependence on target atom and exit angle)

Rutgers group (Busch, Doctor thesis)

Also Marion & Young, calculations



General form for effective ion survival probability as function of energy *E* based on available data (lines, Bailey):

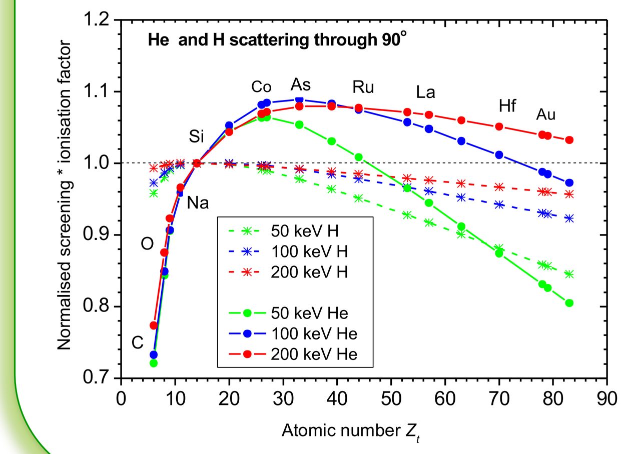
$$P_{ion} = 1 - e^{-\alpha E} \qquad (13)$$

For H: α = 0.019 /keV
For He α = 0.0064 /keV

***P**$_{ion}$* **for for H⁺ & He⁺ ion scattering through 90°** (at the surface) **as function of target atom number Z_t**
Also 100 keV He from depth 40nm

Combined Screening & Neutralisation correction

Combining the screening and neutralisation corrections gives correction curves for the Rutherford X-section as a function of target atom number, normalised to 1 for Si

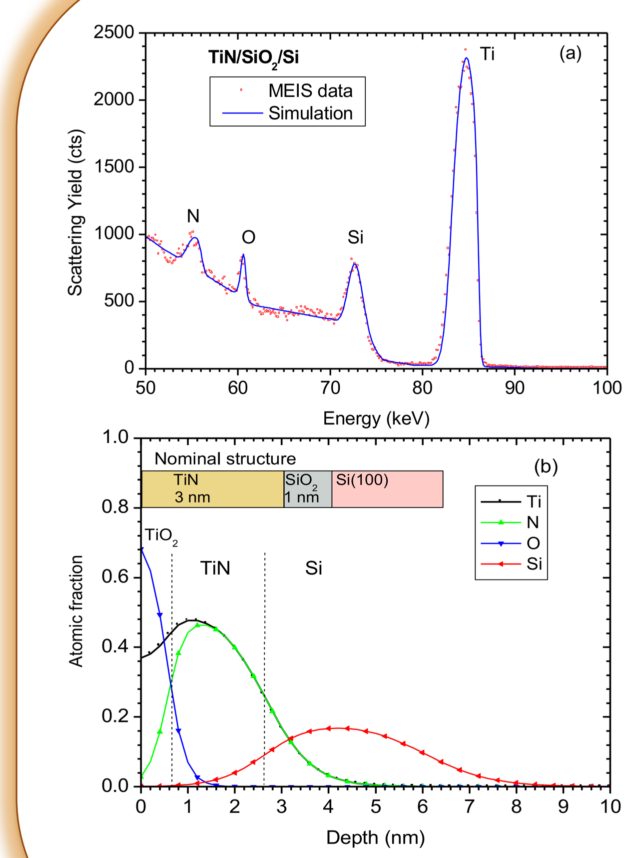


Correction curves for 50, 100 and 200keV H^+ & He^+ ions scattered through 90° (at surface) off target atom number Z_t

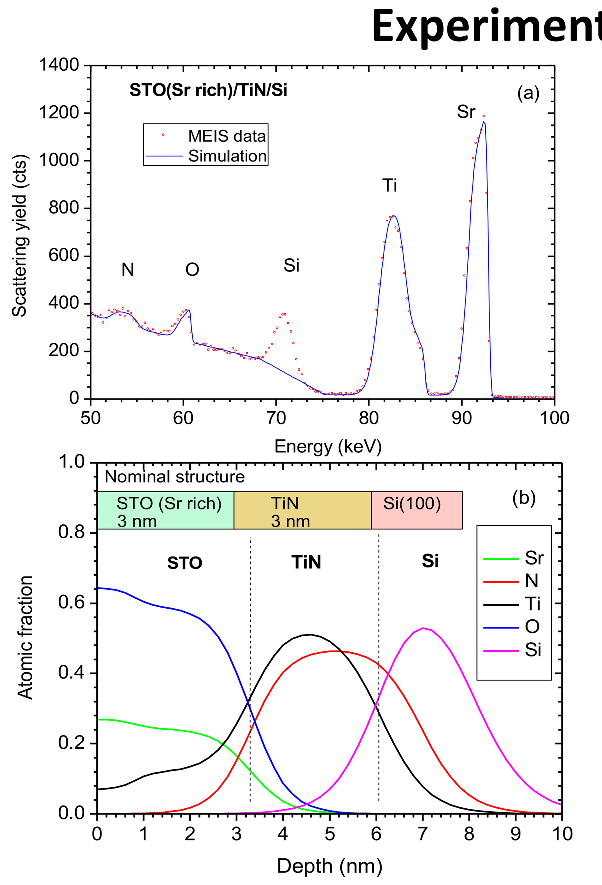
For H: correction ≲10%
For He: correction ≲20%

Overall correction is mass and energy dependent and needs to be included to yield quantitative data.

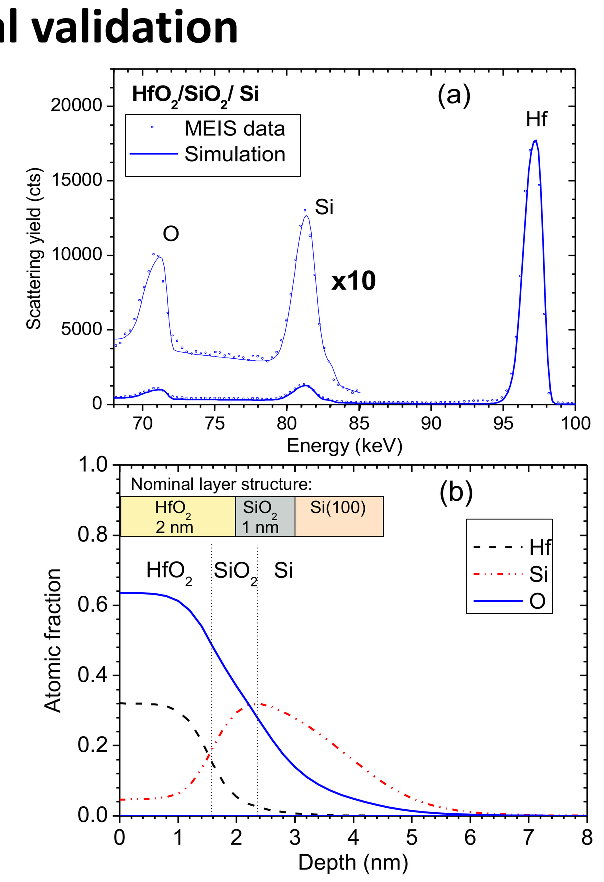
Experimental validation



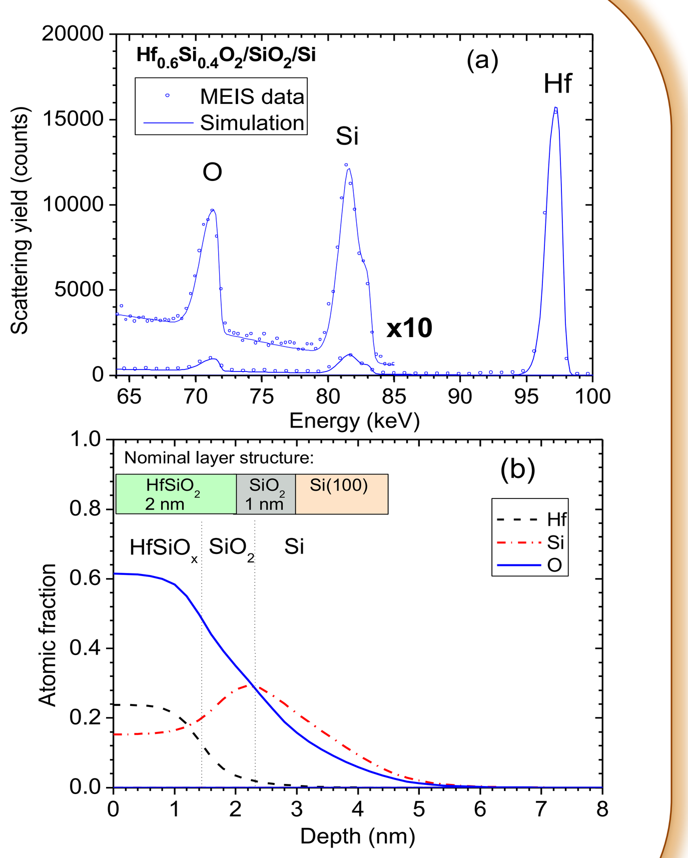
TiN layer: 2.6 nm;
Ti:N = 1:1 away from top oxide



STO layer: 2.3 nm; TiN layer: 2.9 nm
Sr/(Sr+Ti) = 0.6 cf. RBS: 0.62



HfO_2 layer: 1.6 nm - 1.75 nm
Hf:O = 1:2 stoichiometric (≤ 2%)



$HfSiO_2$ layer: 1.4 nm - 1.6 nm
Hf:Si = 0.6/0.4 (≤ 2%)

Spectrum simulation & Experimental confirmation

More complex layer systems can only be effectively interpreted using computer simulation of spectra. The simulation model used at IIAA, based on the IGOR graphing software incorporates the corrections considered above. Its outputs are the fitted spectra and best fit depth profiles of species in a layer. In all cases depth scales have been used which require assumptions re the correct densities of atom species.
Layer thickness and composition compare well with reference data, as shown ↵

Conclusions

- the **MEIS yield ratio** of particles scattered off surface atoms to those at depth x **is given by the Rutherford E^{-2} prediction * the inverse ratio of the particle exit energies to a power B.**
- The impact of screening of the potential on the backscattering yield in MEIS has been evaluated for H^+ and He^+ ions at different energies using the Andersen approach. For a fixed beam energy the **screening correction depends mainly and almost linearly on Z_t**
- Using **experimental neutralisation data** convolved with the **screening correction** leads to a **correction factor to the Rutherford backscattering cross section ratio.** Its dependence on both projectile energy and the atomic number of the scattering atom is presented.
- This **approach has been validated** for a number of representative examples that yield quantitative depth profiles derived from MEIS spectra of nanolayers.
- Although absolute quantification especially when using He ions, may not always be achievable, relative quantification in which all species in a layer add up to 100%, is possible.

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