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23 - 27 February 2009

IBA IX Beyond single scattering off flat samples

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Beyond single scattering off flat samples

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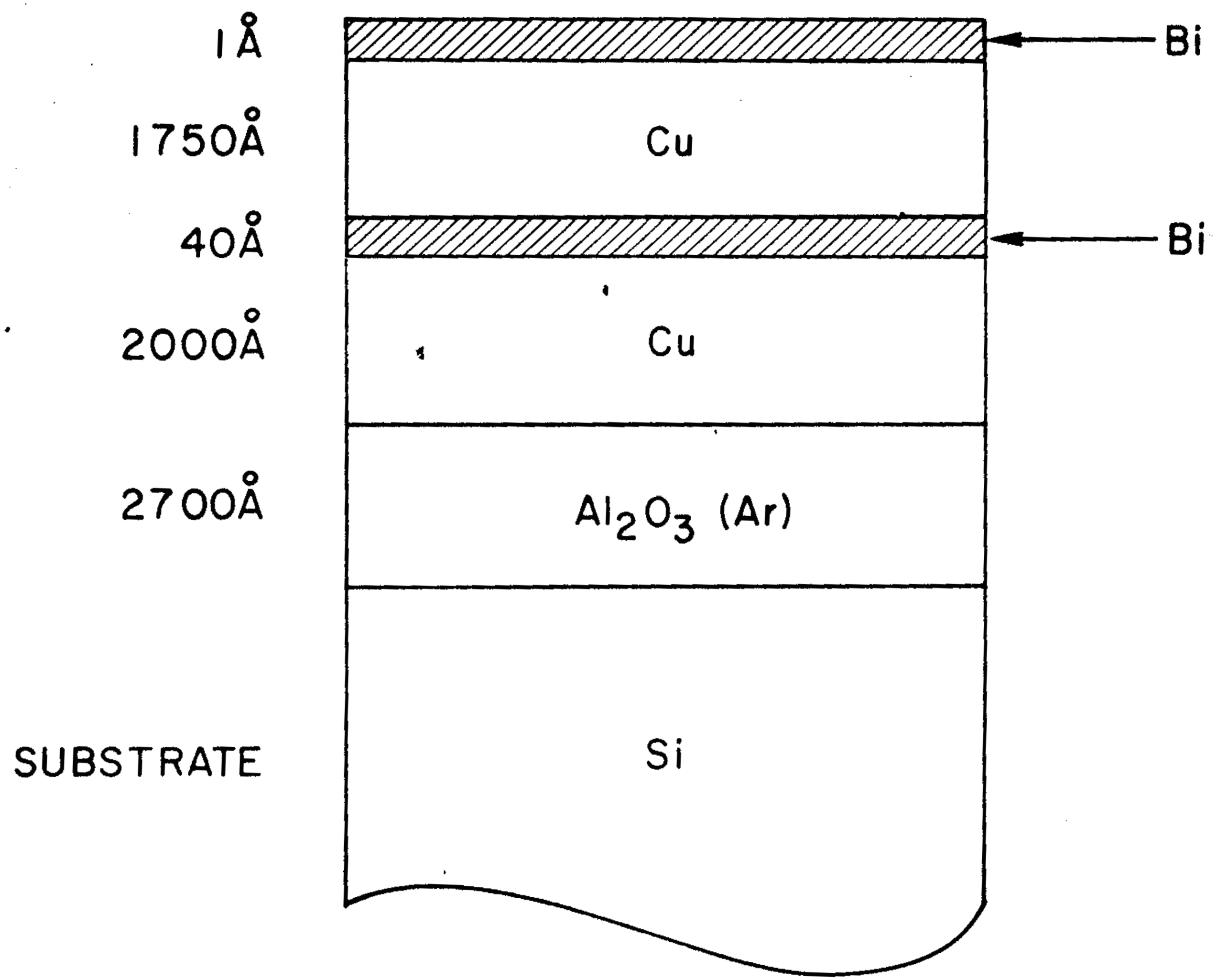
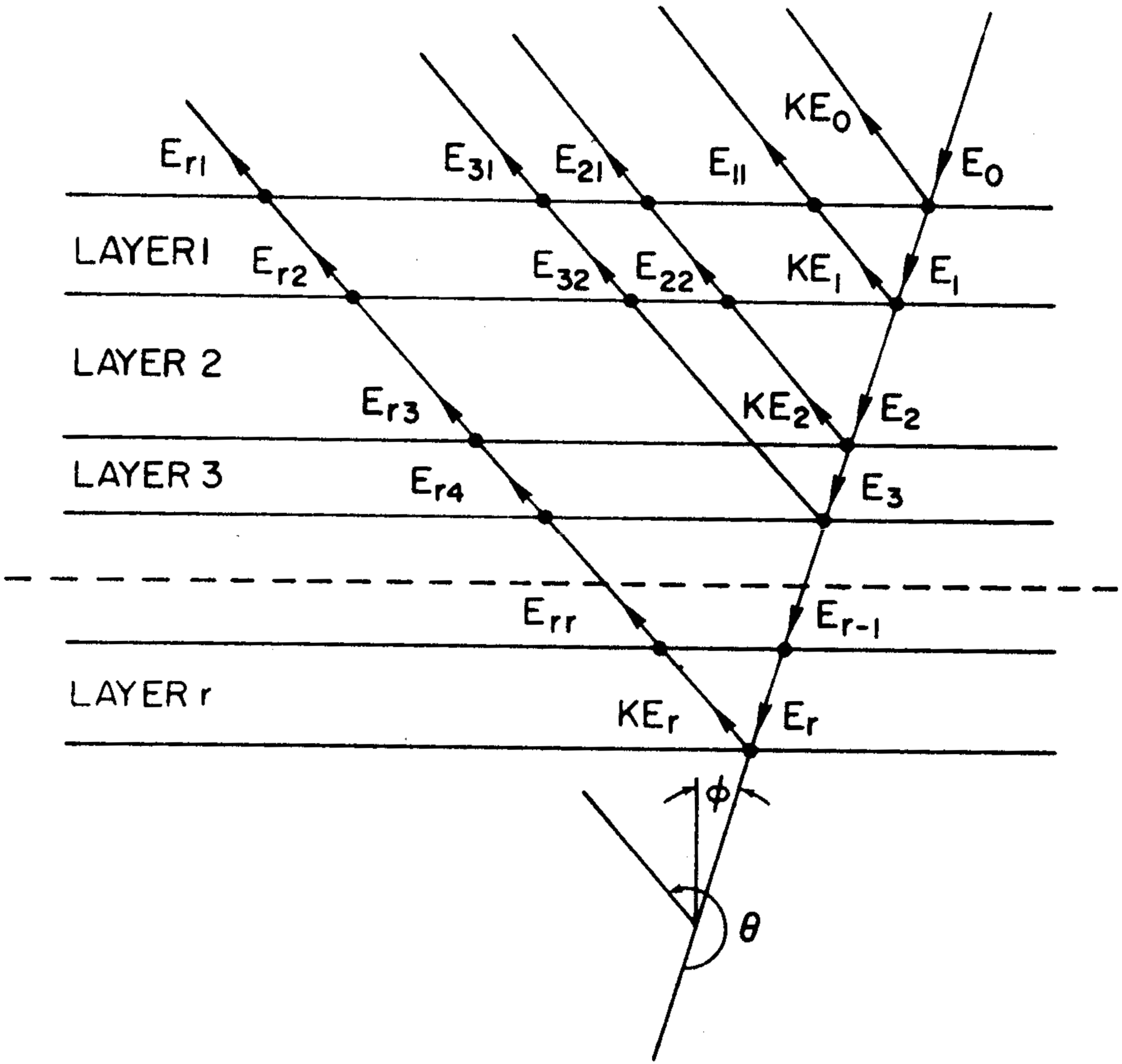
Overview

- Introduction: “Clean” vs. “dirty” RBS
- Roughness and 3D structures
- Sources of background
- Shape of signals – some effects
- Multiple scattering – some effects

Computer-aided analysis: “clean” RBS



J. F. Ziegler et al., Proc. 2nd Int Conf on IBA (1975)


KE0
E0
Er1
E31
E21
E11
LAYER1
Er2
E32
E22
KE1
E1
LAYER 2
Er3
KE2
E2
LAYER 3
Er4
E3
Err
Er-1
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φ
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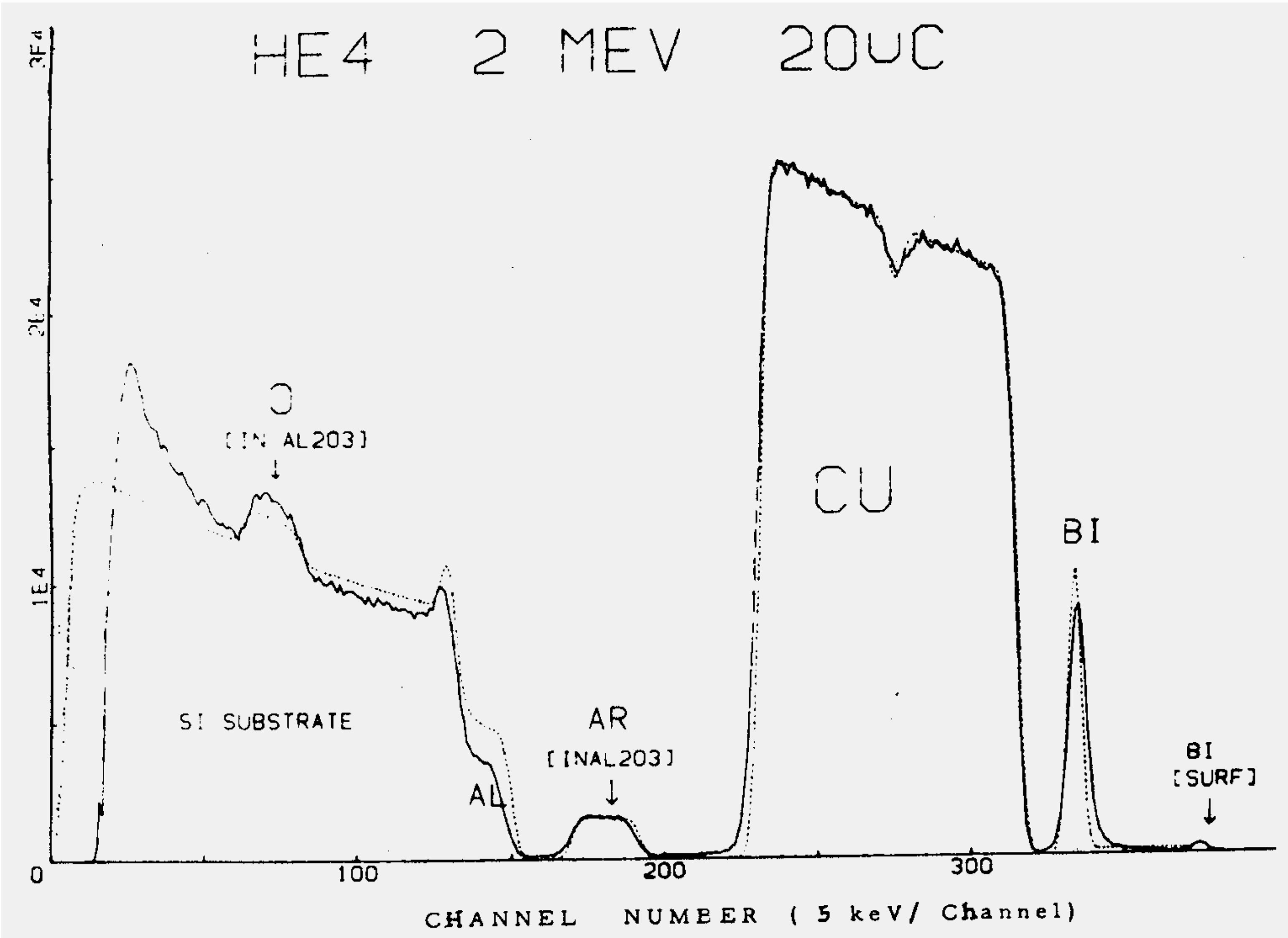
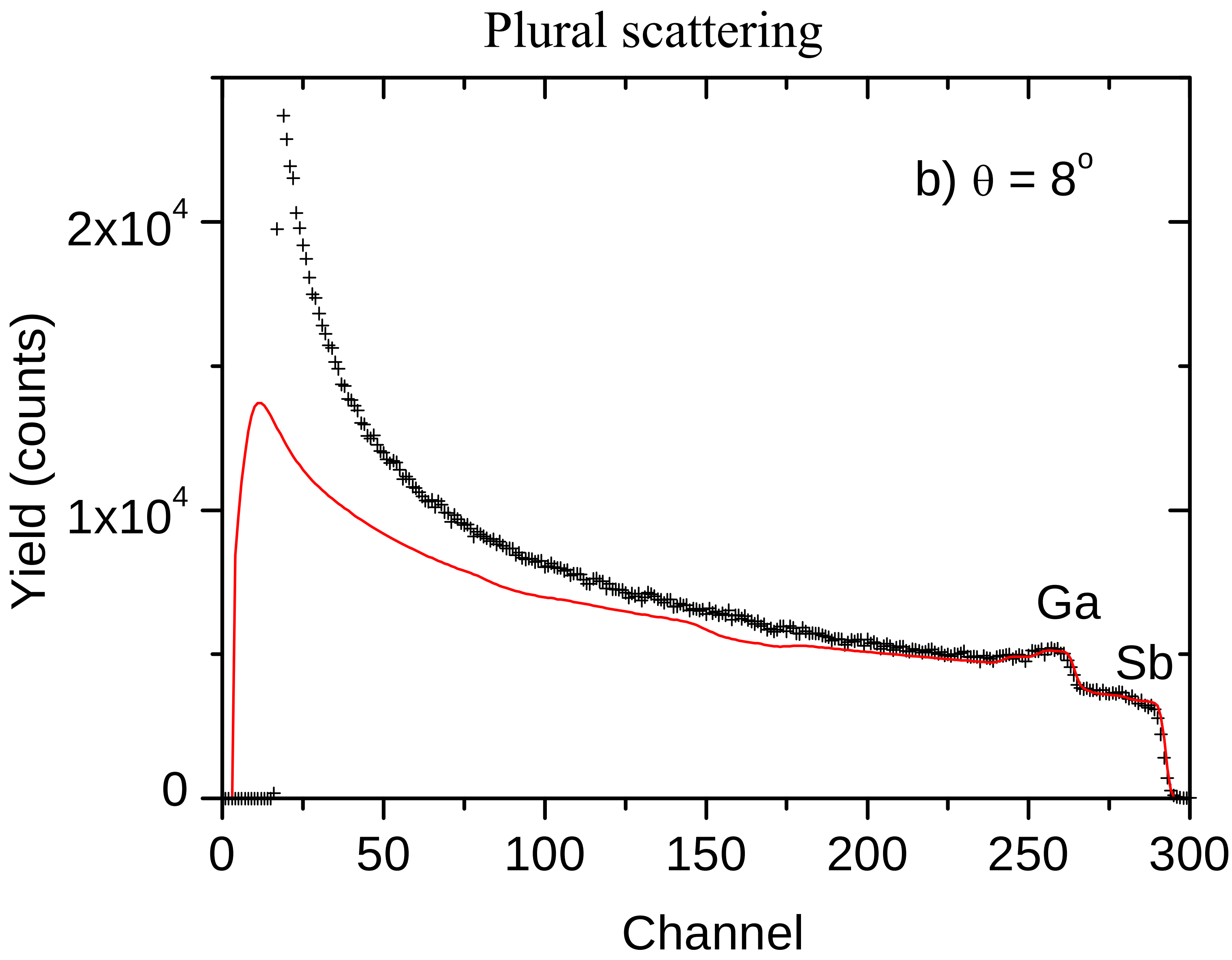
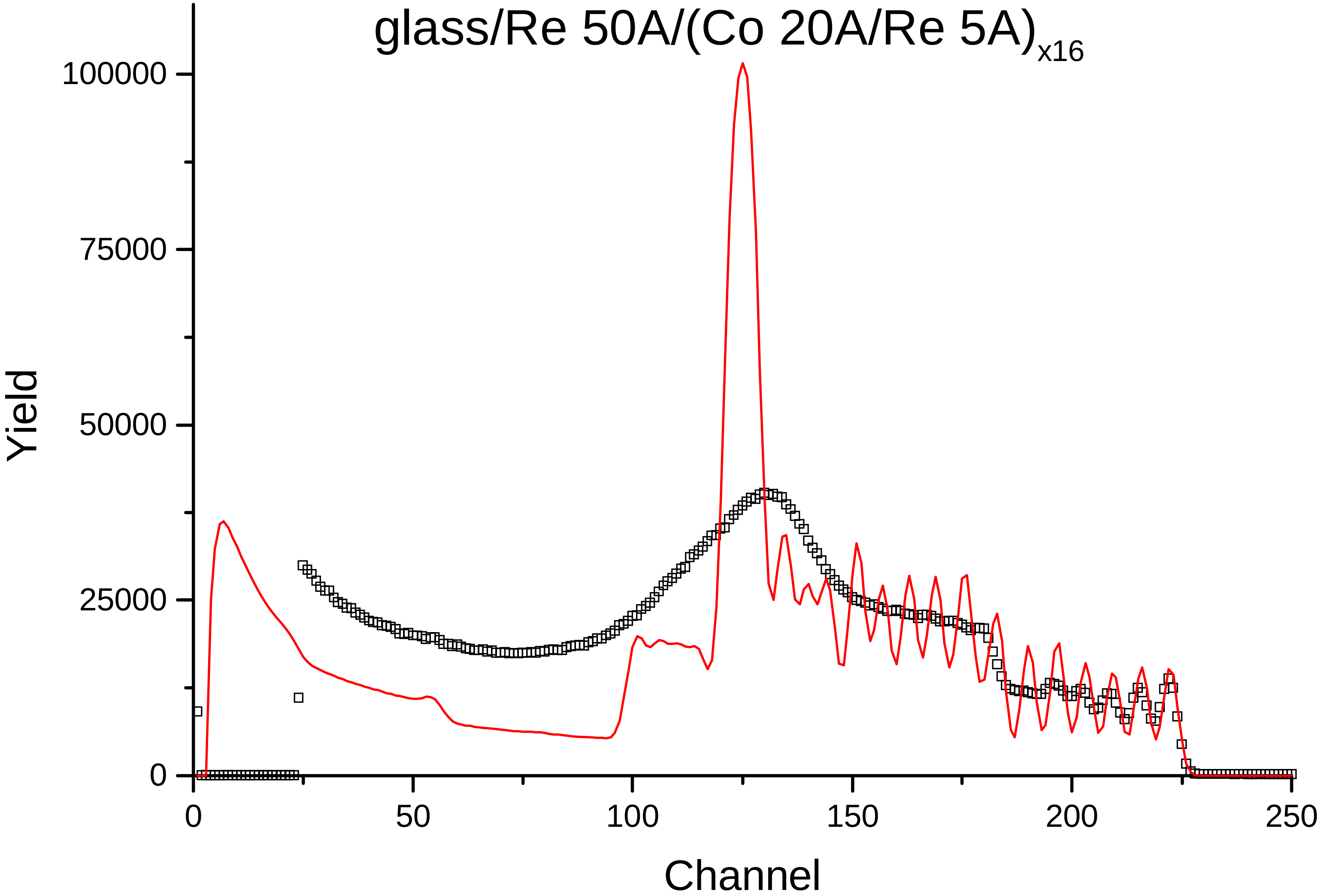


HE4 2 MEV 20uC
3E4
2E4
1E4
0
O
[IN AL2O3]
SI SUBSTRATE
AL
AR
[INAL2O3]
CU
BI
BI
[SURF]
100
200
300
CHANNEL NUMBER (5 keV/ Channel)

Calculation may not be good enough!



Multiple scattering



What can we do?

- Rely on experience of "experienced user"
- Monte Carlo calculation of all known effects (still has some difficulties!)
- Include known effects in analytic model as thoroughly as possible

“Dirty RBS”

- Beam-sample interaction
  - Energy loss straggling
  - Plural scattering
  - Multiple scattering
  - Channelling
  - Beam charge state
  - ...
- Experimental system
  - Beam energy spread
  - Beam angular spread
  - Finite size of beam spot
  - Finite size of detector
  - Pulse pileup
  - Slit scattering
  - ...
- Sample
  - Surface/interface roughness/mixing
  - 3D structures
  - Extra elements present, or in unexpected places
  - Undetectable elements
  - ...

Roughness and 3D structures

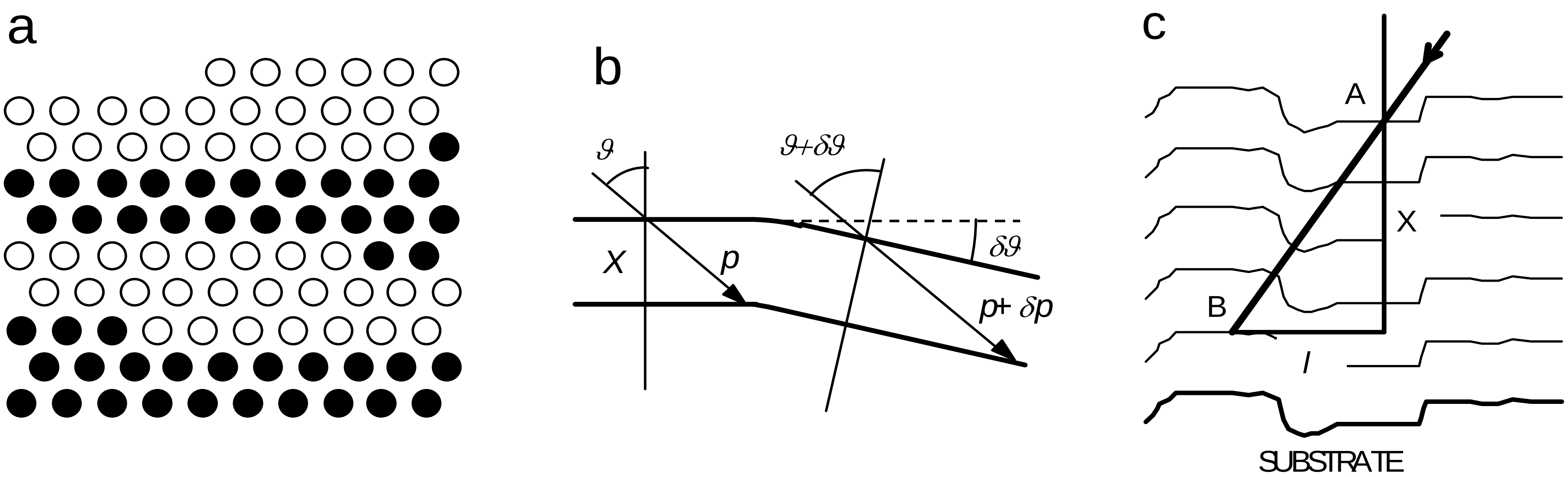
- Surface roughness
- Interface roughness
- Substrate roughness
- Quantum dots, inclusions, voids
- Lateral inhomogeneity
- ...

➢ RUMP: summing of a few structures (fast, pretty useless)

➢ SIMNRA: summing of many structures (excellent, slow)

➢ NDF: effect on signal width (fast, good when applicable)

Roughness - models



The effect of roughness is similar to that of energy straggling: additional broadening of the features present in the energy spectrum

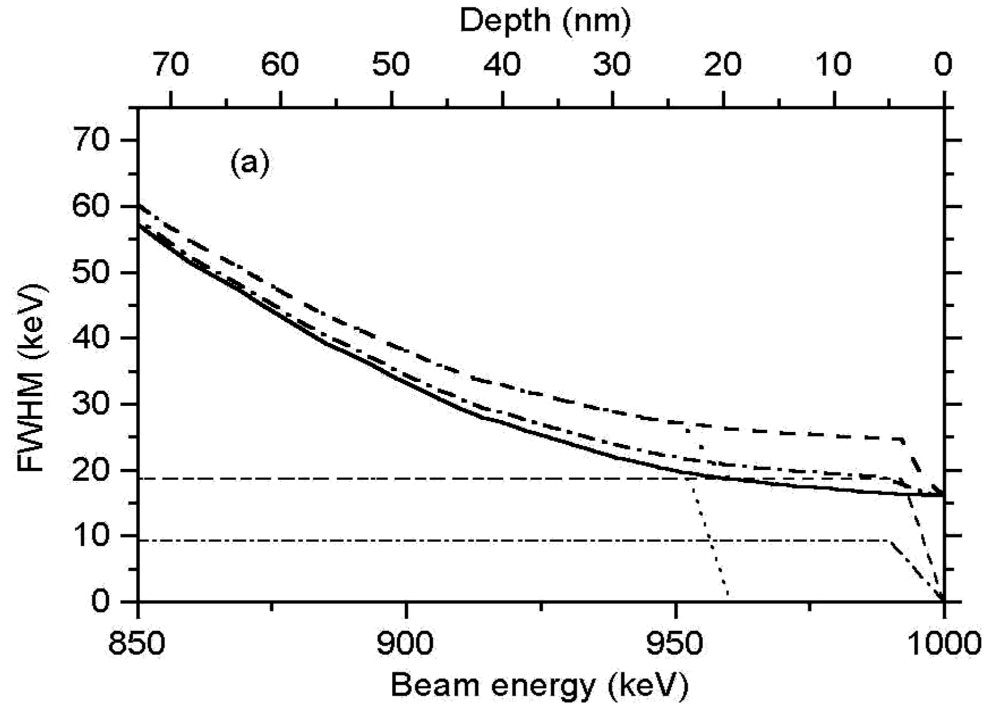
Calculate the broadening due to roughness:

assign it as an extra contribution to the energy straggling

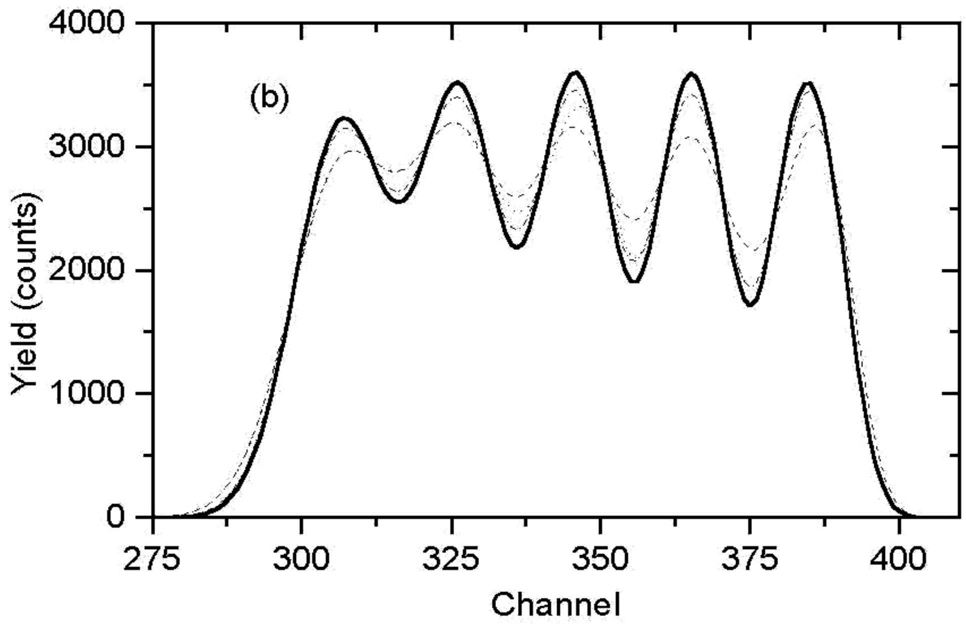
obtain an apparent energy resolution

This is convoluted with the theoretical spectrum in the normal way.

1) Thickness inhomogeneity of a given layer

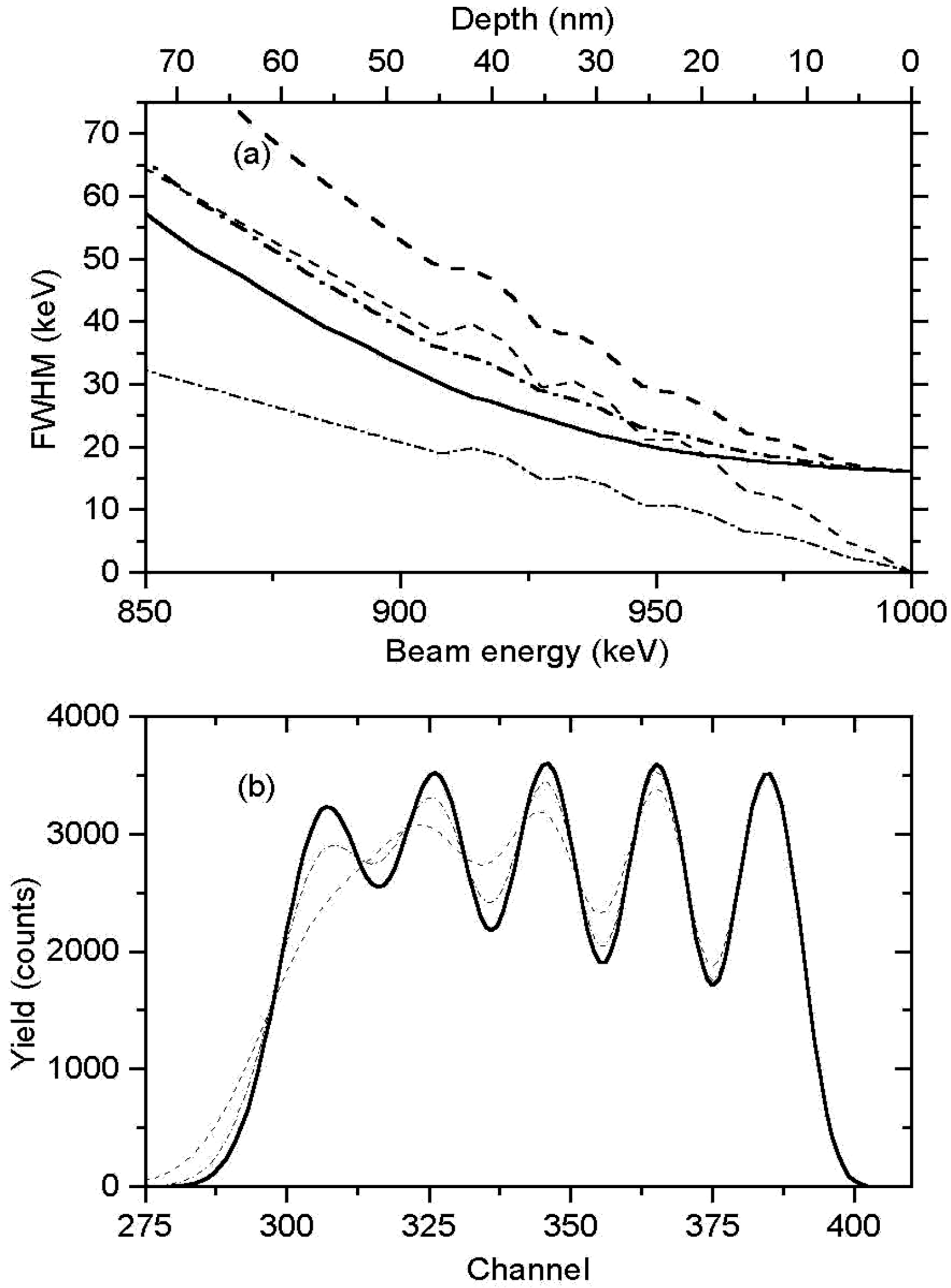


Si/(Si 4 nm/Ge 6 nm)x5



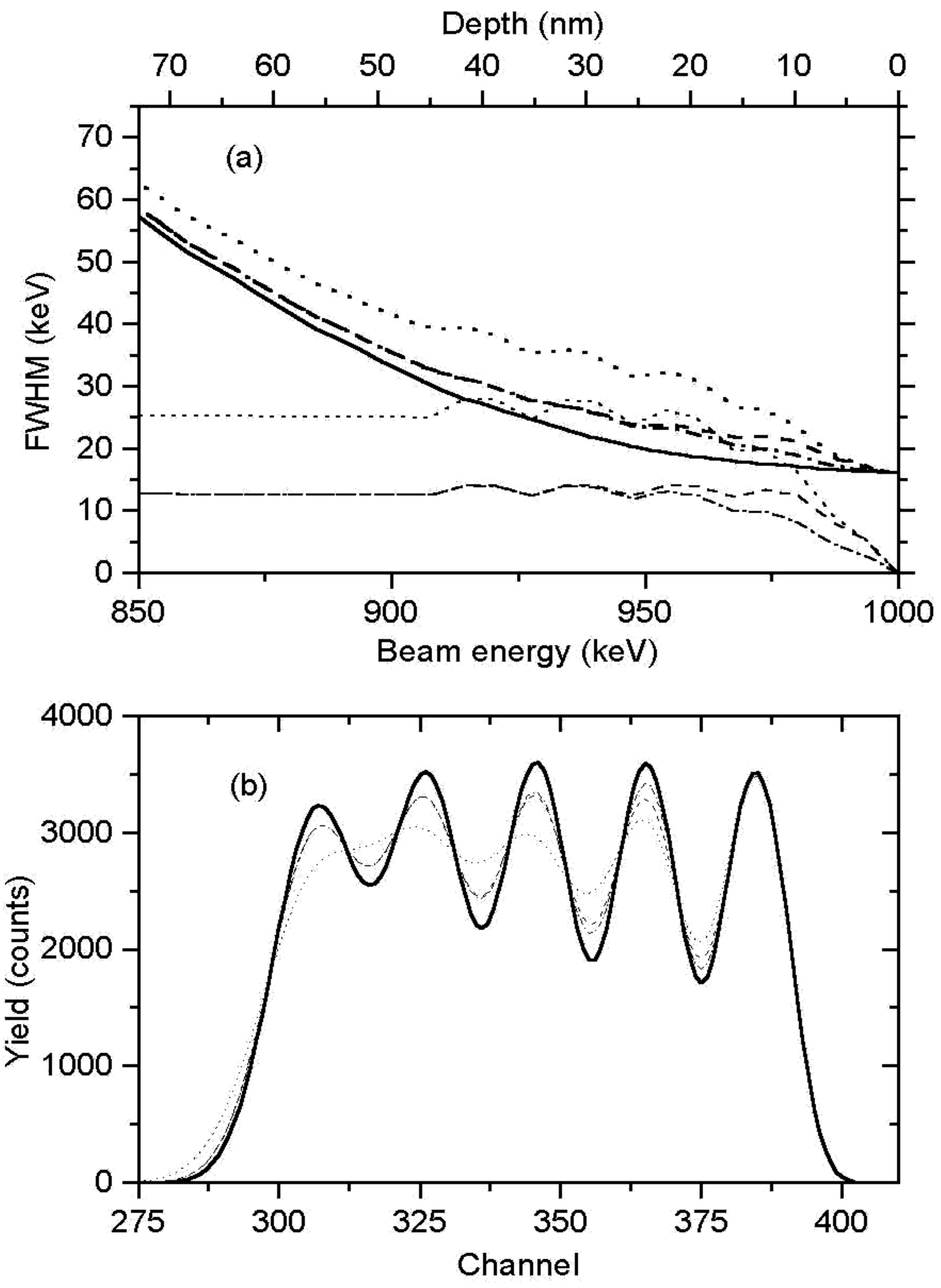
2) Corrugated sample

Si/(Si 4 nm/Ge 6 nm)x5



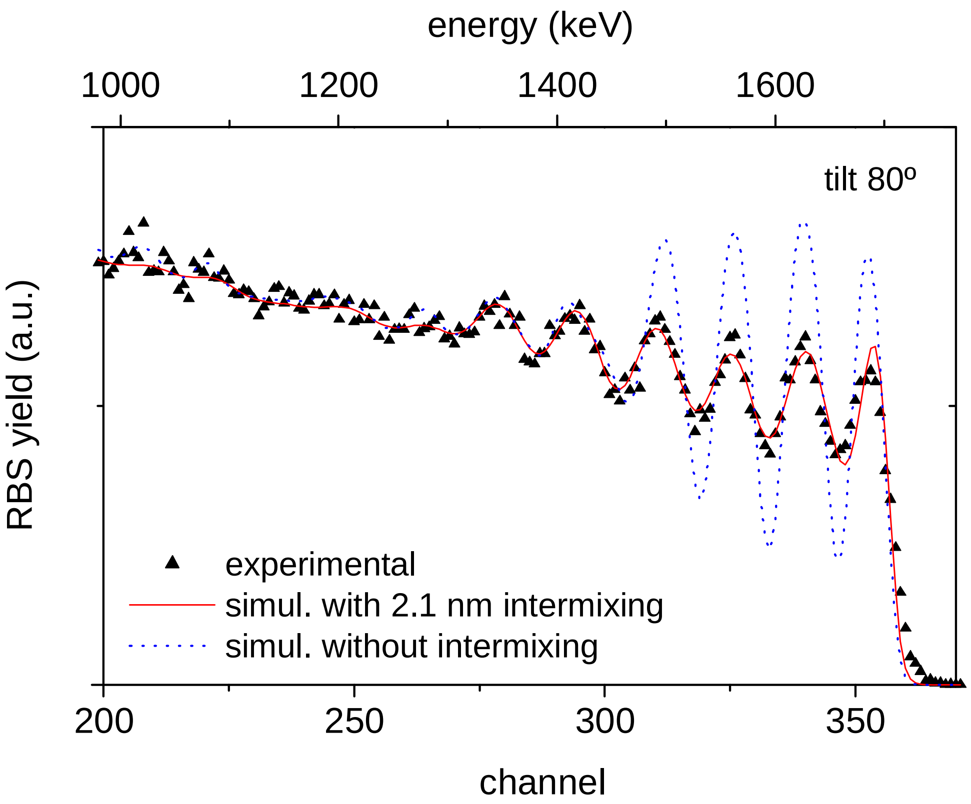
3) Rough substrate surface

Si/(Si 4 nm/Ge 6 nm)x5

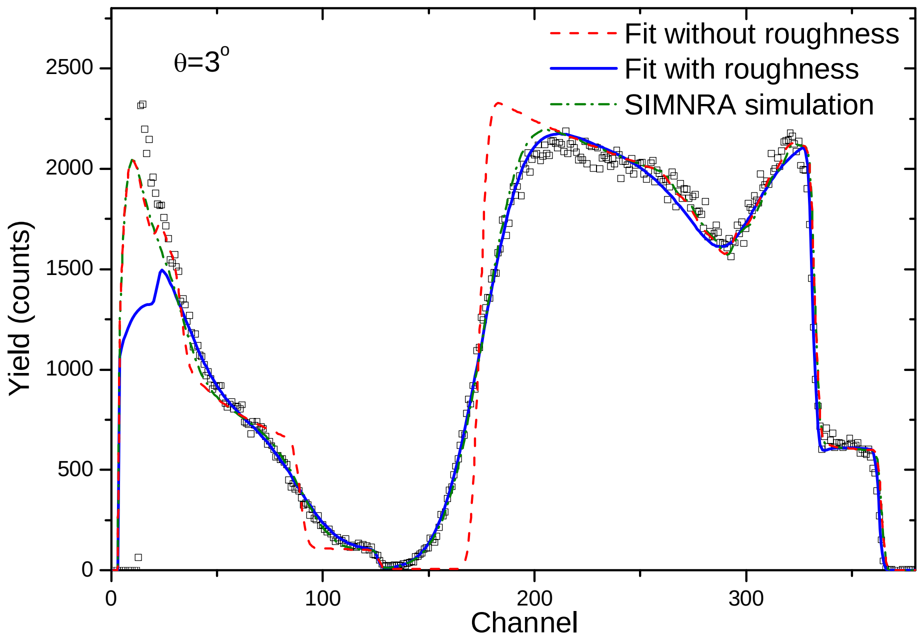


➢ Some examples

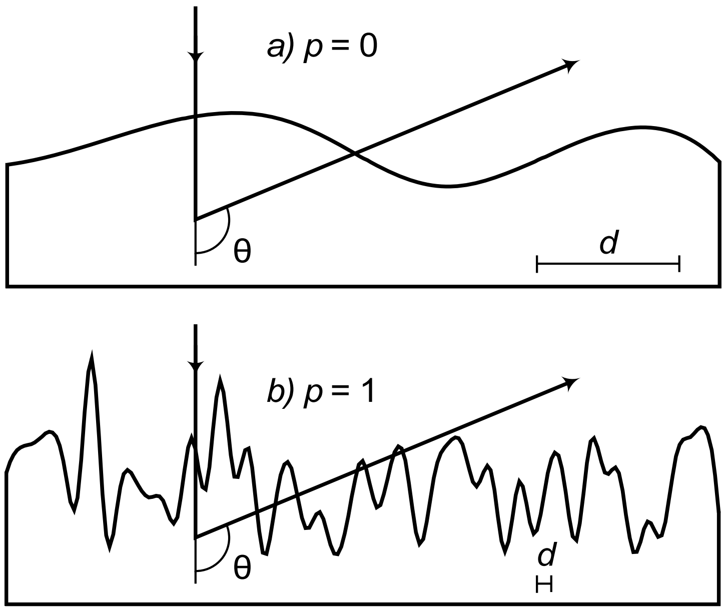
➢ $(Ti_{0.4}Al_{0.6}N/Mo)\times 50$

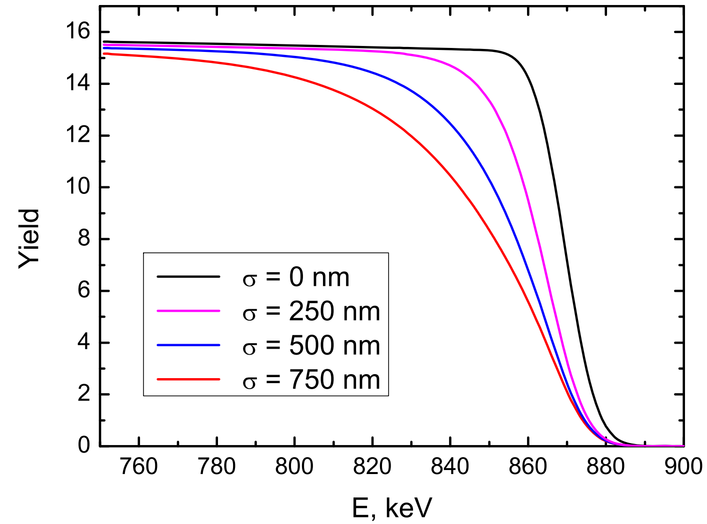


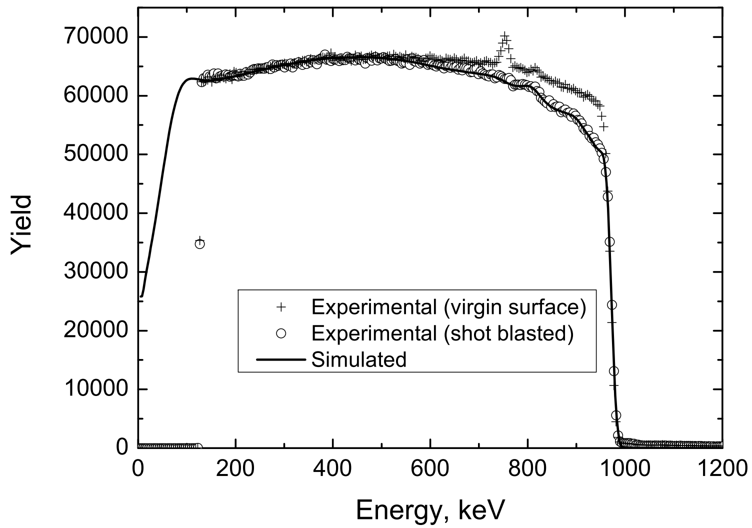
➢ InGaN film on GaN (on alumina)

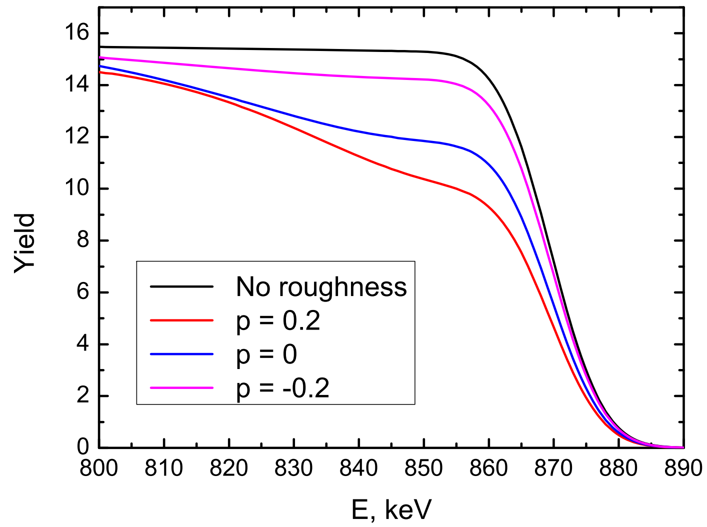


➢ SL Molodtsov, AF Gurbich, C Jeynes, J.Phys D Appl Phys 41 (2008) 205303



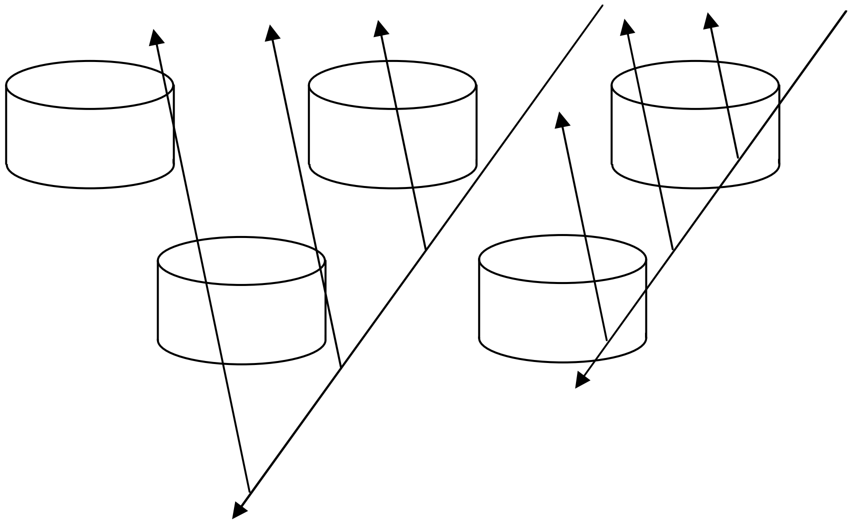






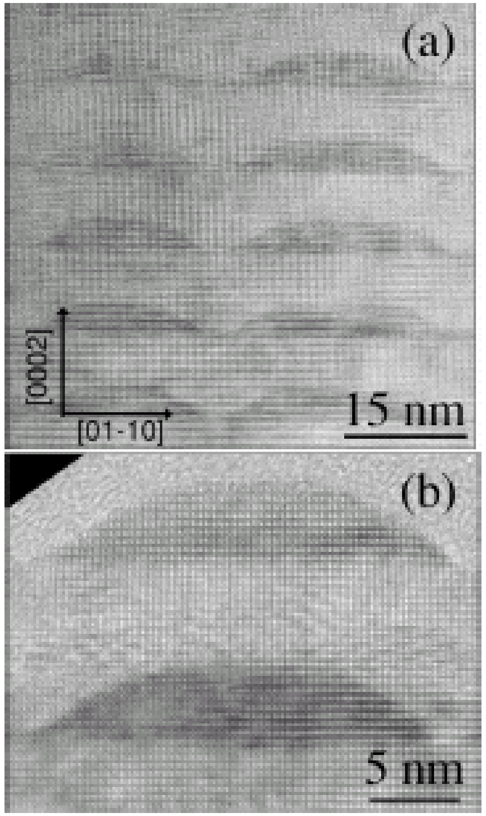
Quantum dots

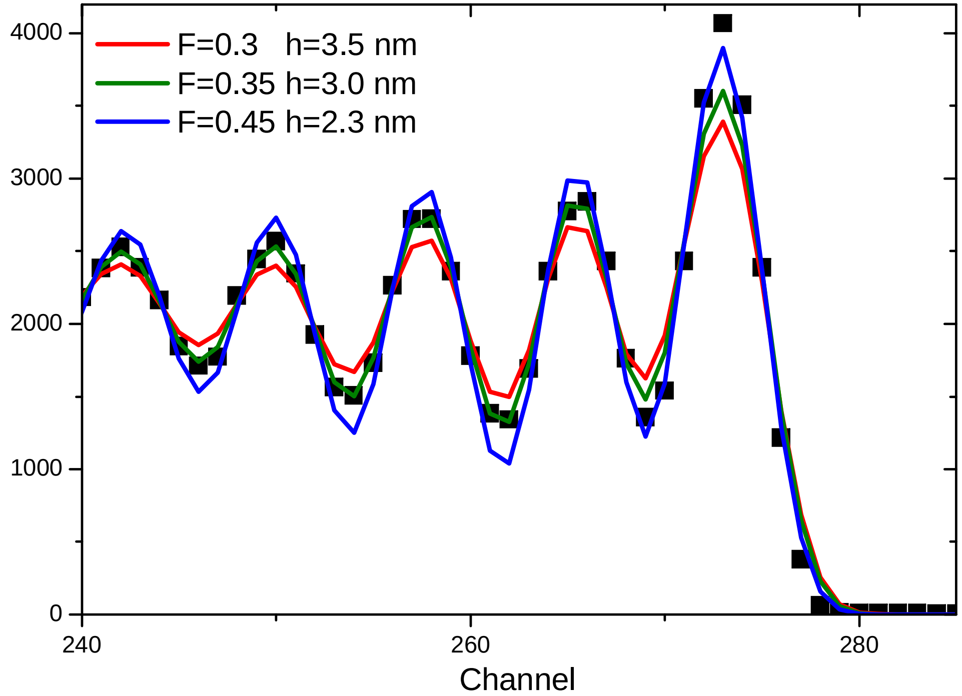
- Quantity of matter is easy to calculate (with automatic creation of sub-layers as needed)
- Extra source of energy spread due to different stopping in QDs :
  - $\Omega_{tot}^2 = \Omega_{system}^2 + \Omega_{straggling}^2 + \Omega_{QD}^2$



- The point is to calculate Ω_{QD}!
  - Spherical inclusions: JP Stoquert, T. Szörényi, PhysRevB 66 (2002) 144108
  - Cylindrical inclusions: developed by NPB

➢ GaN/AlN self-organised QDs





- ➢ Volume fraction of GaN QD: 0.35-0.4
- ➢ Height of QDs: 2.6-3 nm

Quantum dots in NDF

- Known samples can be simulated: good
  - Both total yield and energy spread are included

- Constraints can be put on possibilities: good
  - But complementary techniques are required

Assumptions in roughness models

(a) The beam area must probe a representative sample of the roughness distribution. This condition is in practice always met when using microscopic beams of size typically 1×1 mm^2.

(b) Gaussian distribution of roughness parameters. Other types of distributions (for instance, surfaces or interfaces with periodic structures) are not correctly modelled.

(c) The beam does not re-enter the sample. Structures with large aspect ratio cannot be simulated with this method.

New work by Molodtsov et al. removes this assumption; still not implemented in data analysis codes: soon!

(d) Roughness parameters must be within well-defined range.

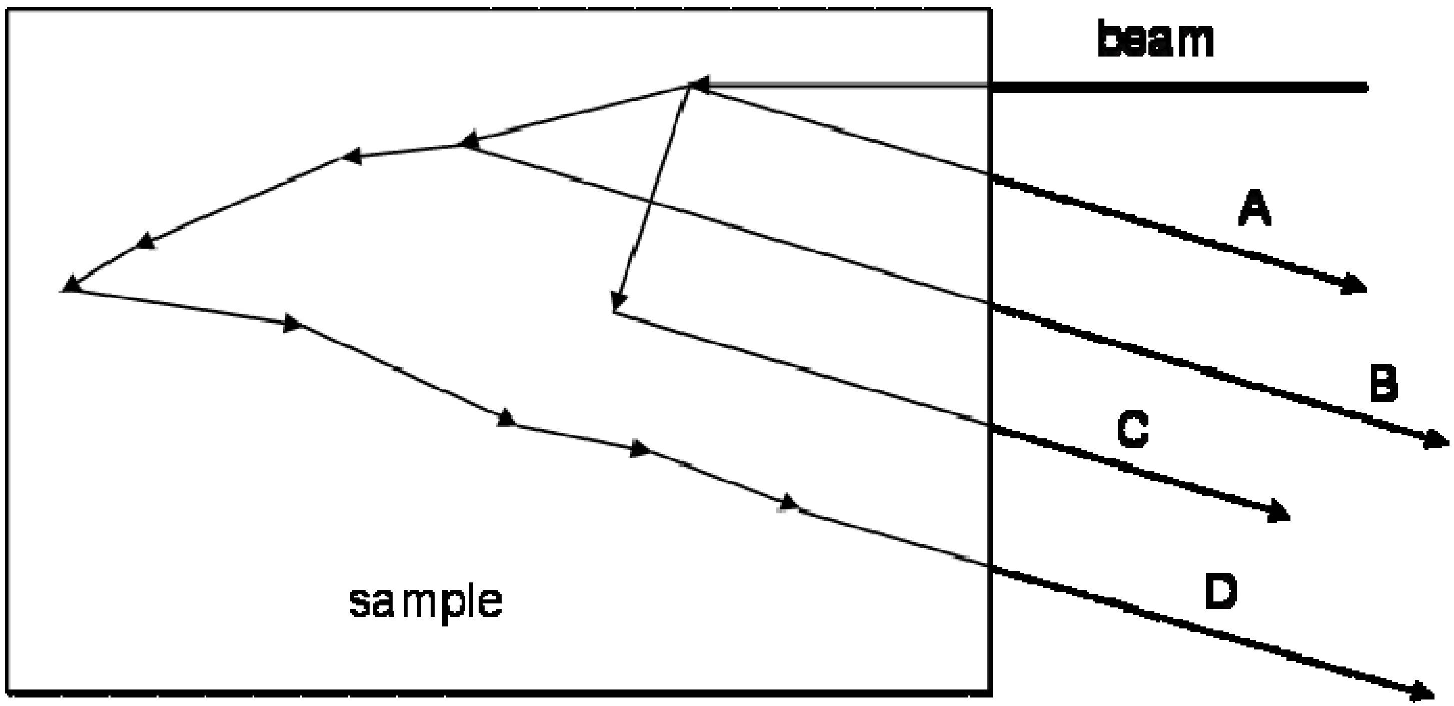
Sources of background

- Plural scattering
- Pulse pile-up
- Slit scattering
- Some effect not yet understood?

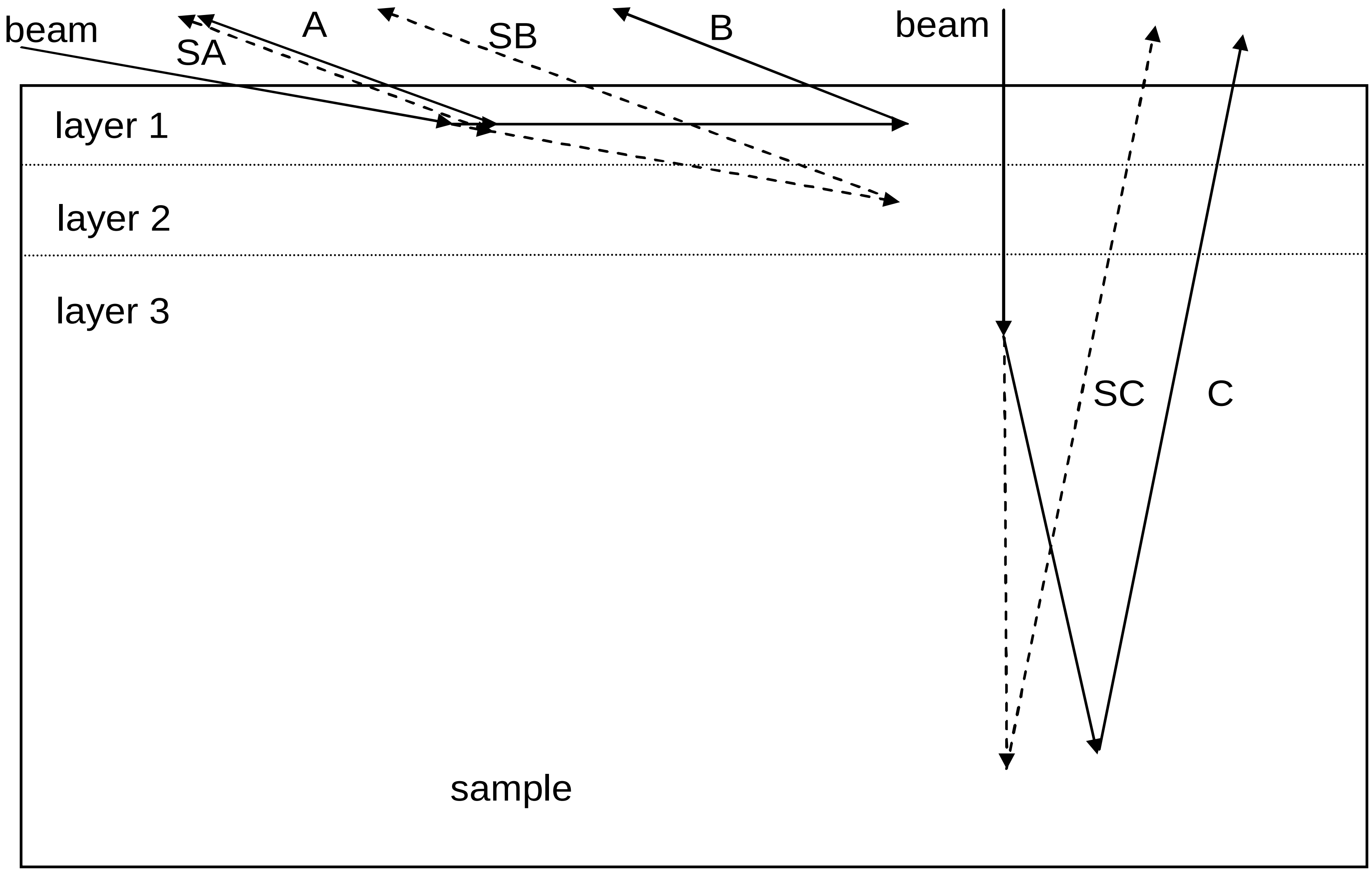
- Leads to reduced sensitivity to small isolated signals
- Leads to distortion of the signal that must be accounted for in accurate simulations

Sources of background

- Plural scattering



➢ Traditionally, an ad-hoc cut-off angle ≈20º has been imposed.

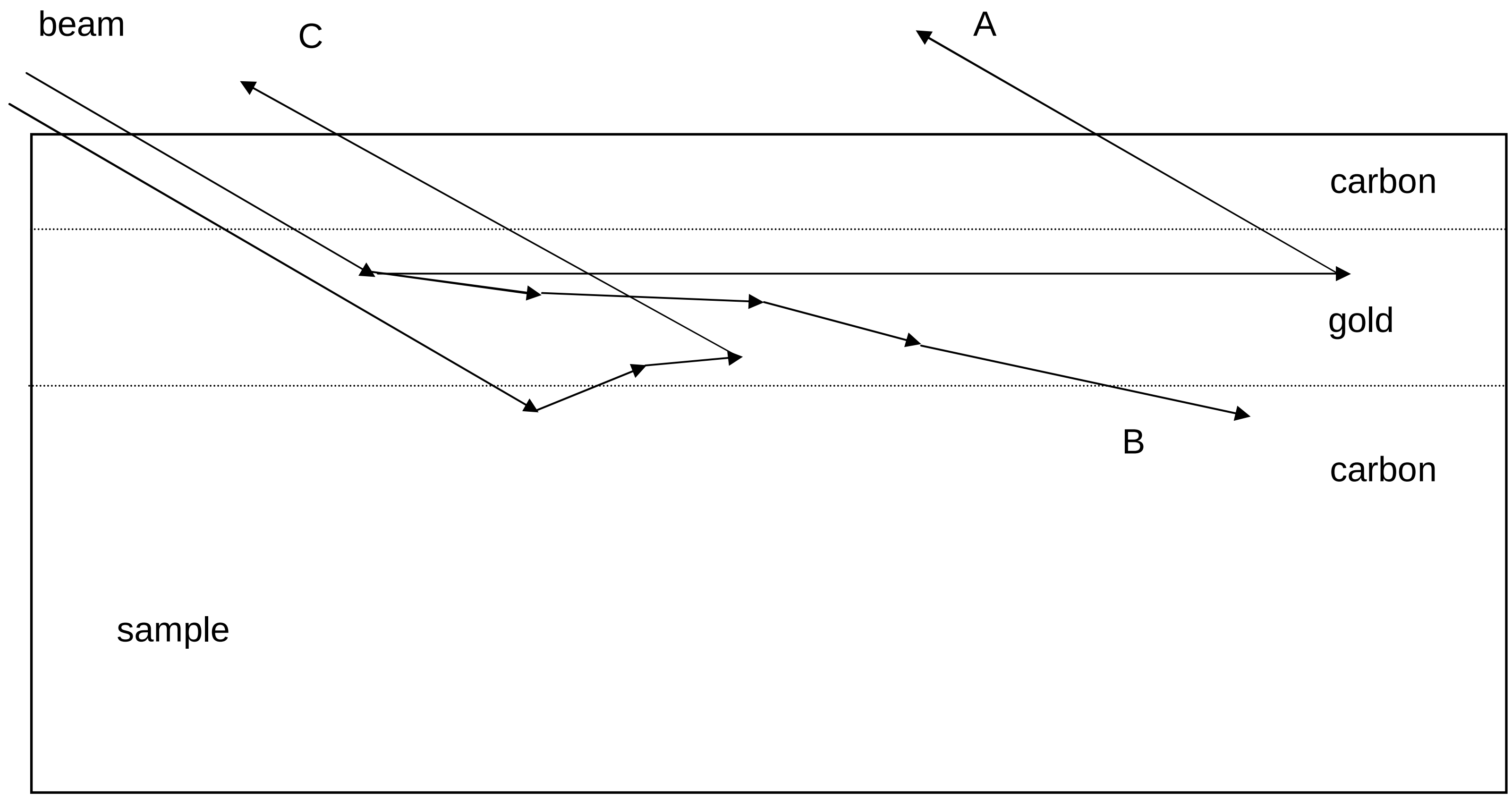


- Cut-off angles do not work at grazing angle!
  - Actual trajectories must be considered.

➢ Model implemented in NDF

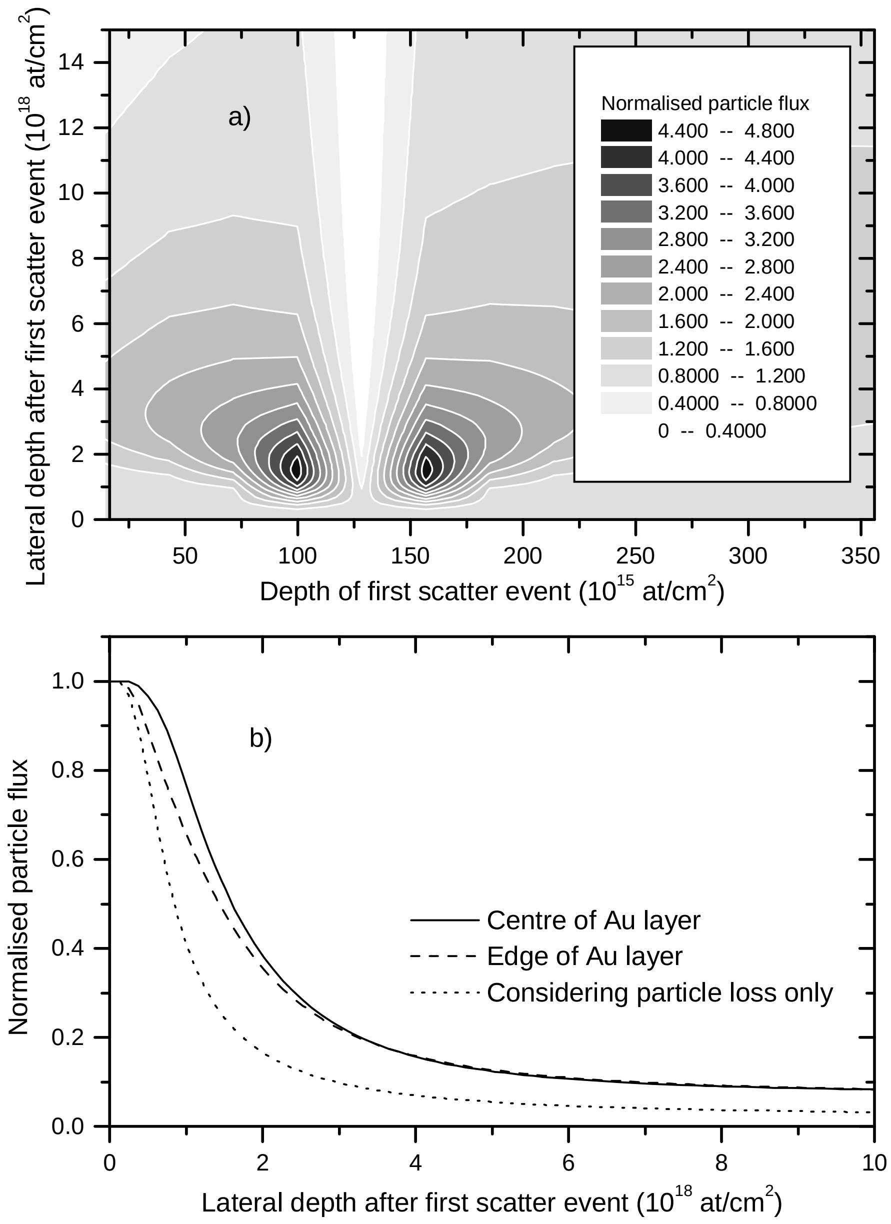
- ➢ Take all events where both scattering angles are larger than 20º
- ➢ Otherwise, take events where trajectory changed more than 50% compared to the corresponding single scattering trajectory. Values between 25% and 100% lead to similar results.
- ➢ Reject events with scattering angle < 1º (to avoid the singularity at 0º; such angles are never used in RBS anyway).
- ➢ Use a large number of different directions after the first scattering (up to 5000).
- ➢ Use a high density of trajectories in regions with high cross sections
- ➢ For speed, reject the trajectories that all together carry only 1% of the cross section (which can be the majority!).
- ➢ Consider influence of lateral spread.

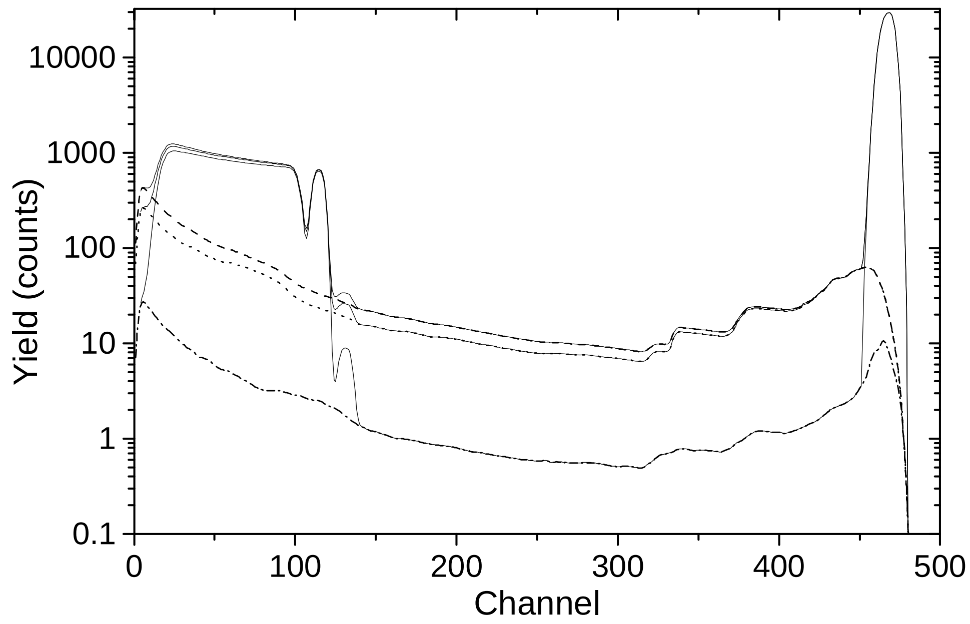
➢ Influence of lateral spread



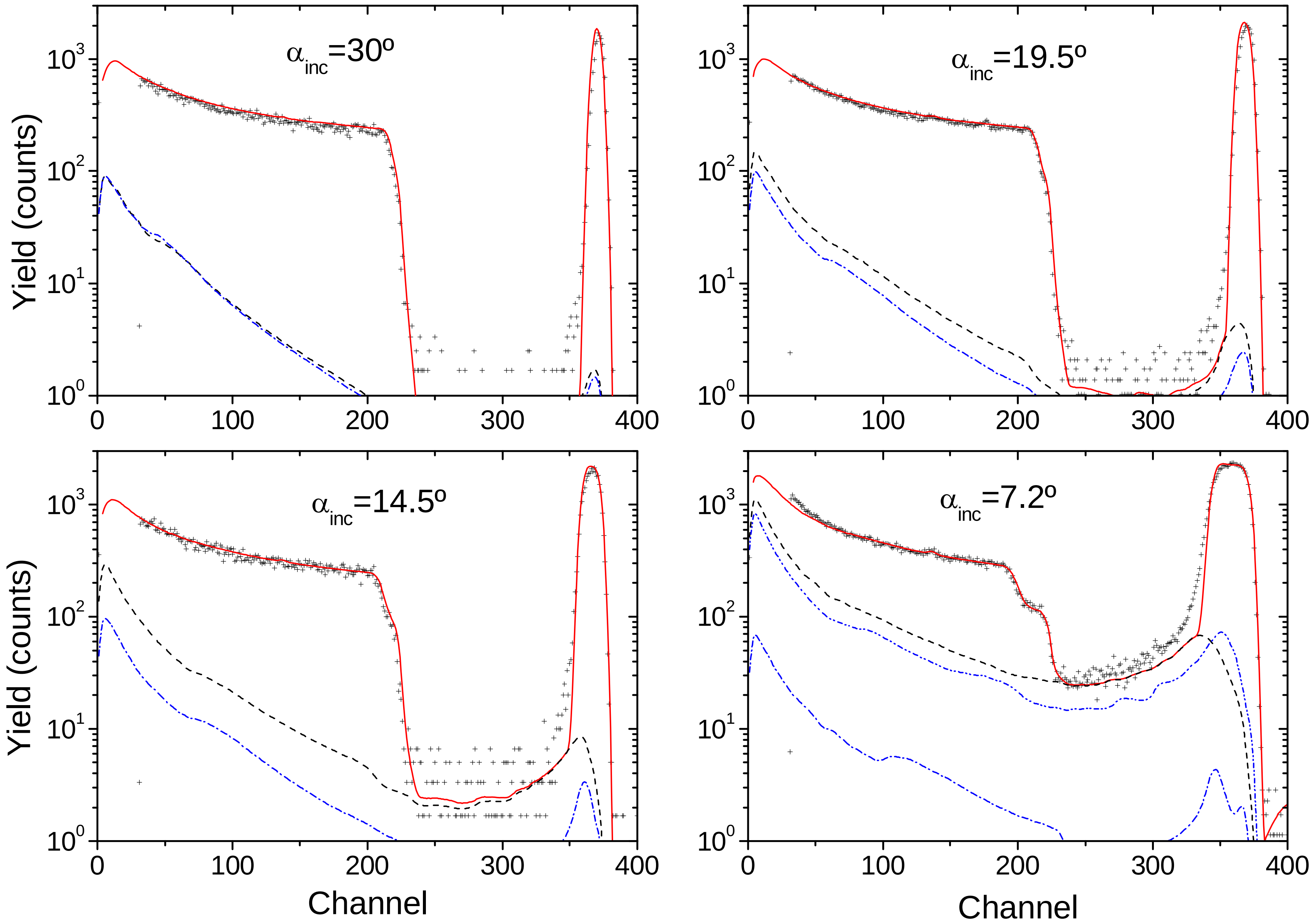
➢ Effective reduction of flux in high-Z layers

➢ Use model of Amsel et al. to calculate lateral spread

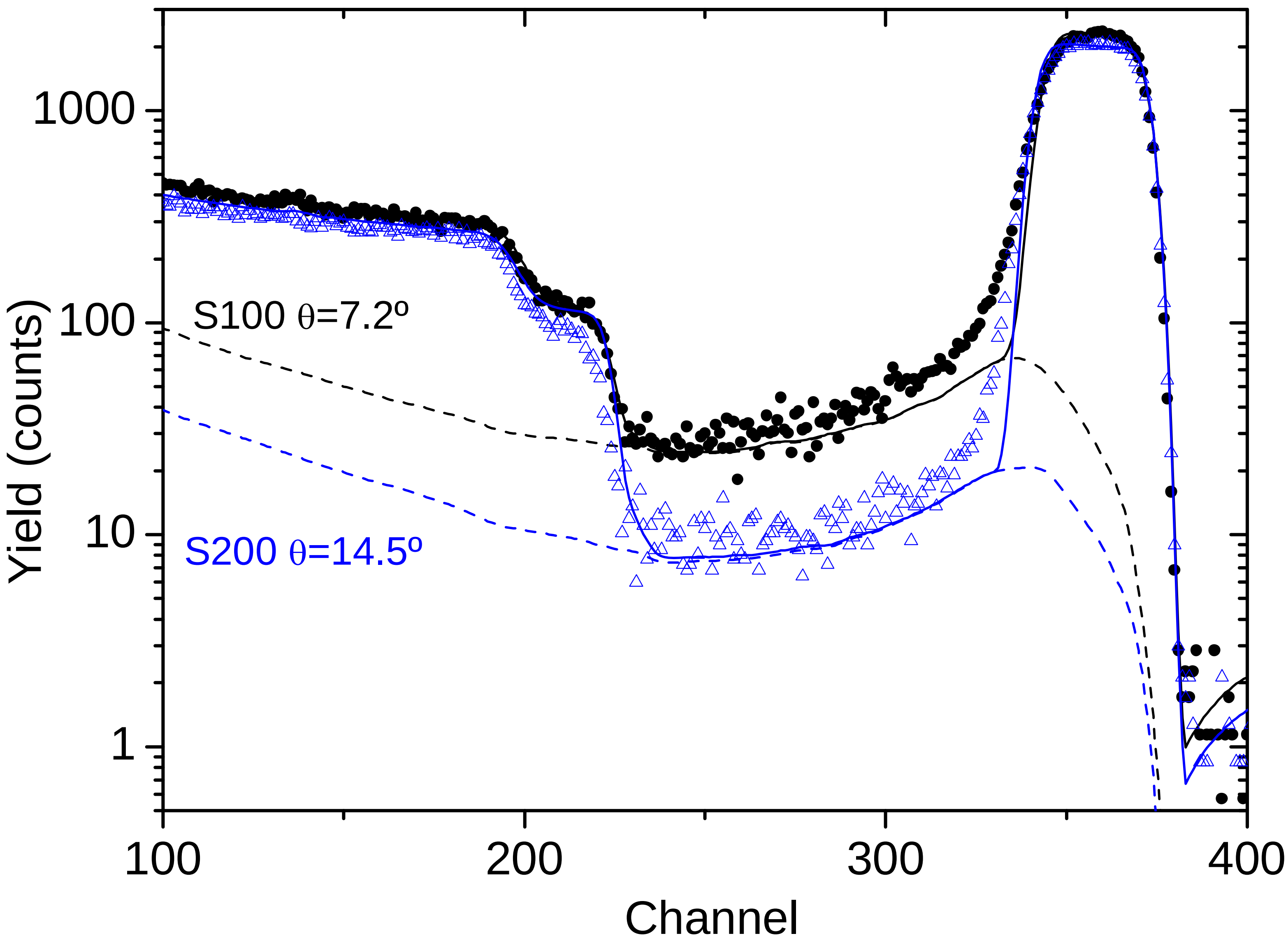




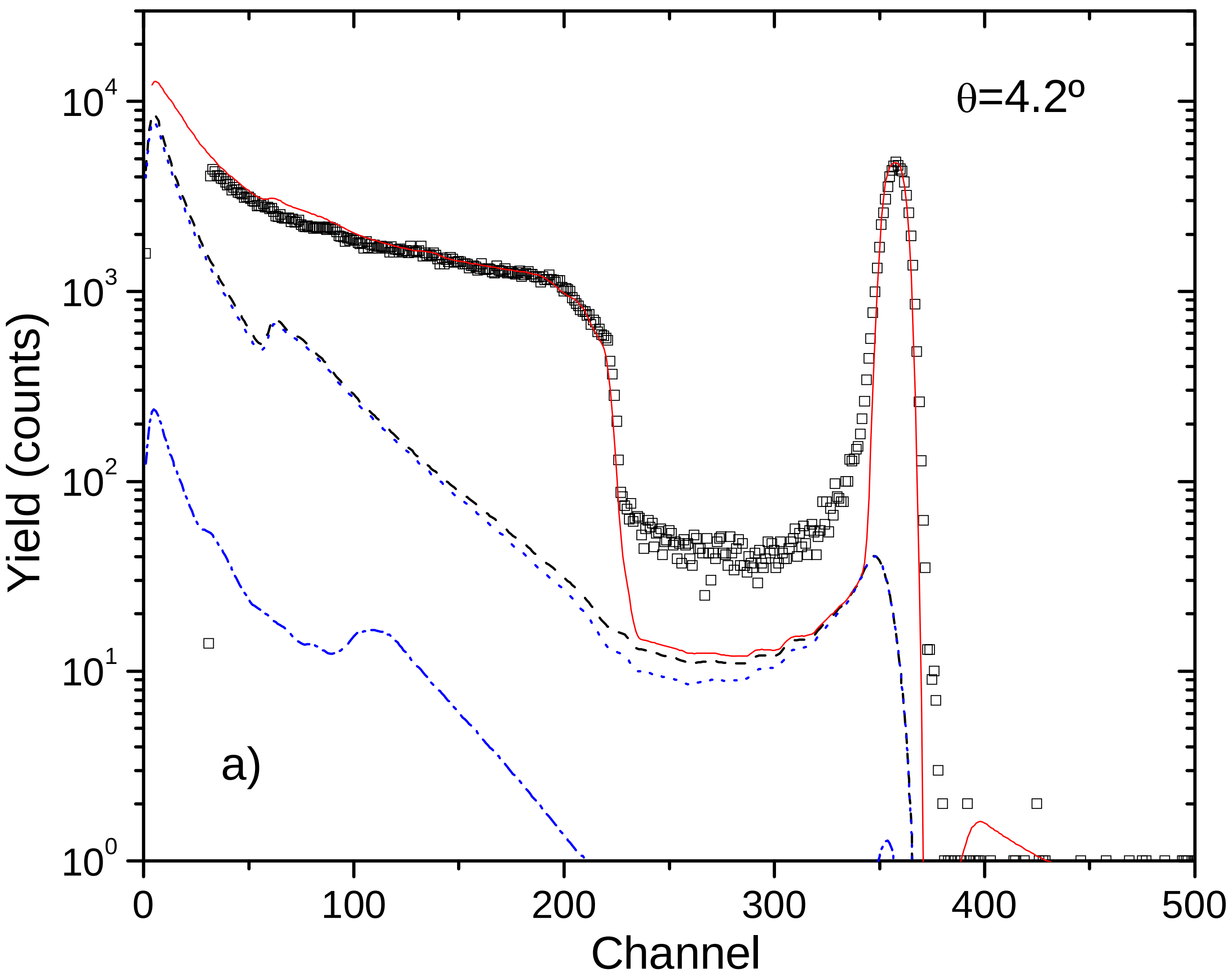
➢ Results: Si/PtSi 48×10^{15} at./cm^2



➢ Results: same nominal path (80 nm ot PtSi)



➢ Results: where the model fails



➢ Si/PtSi 7×10^{15} at./cm^2

Sources of background

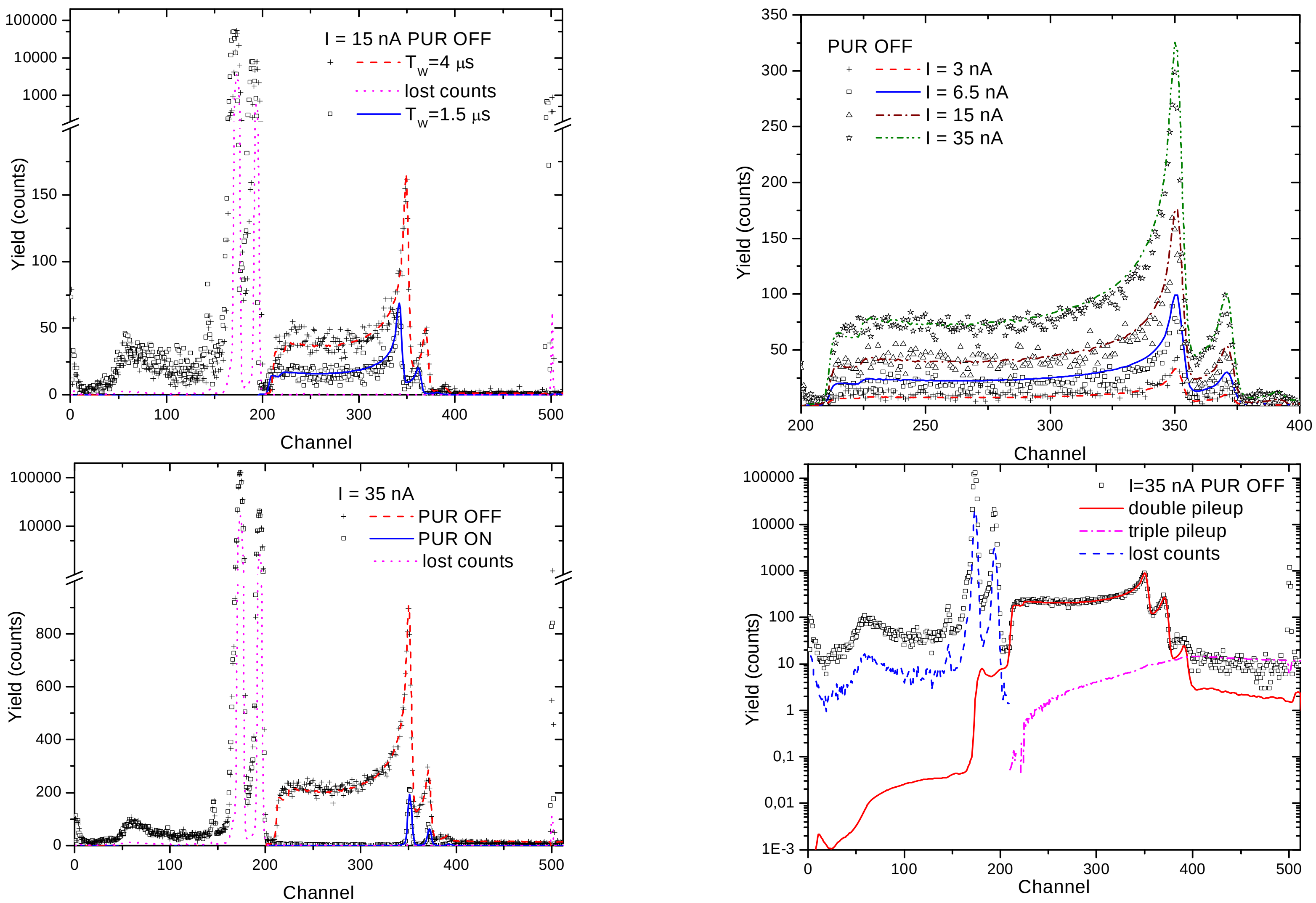
- Pulse pile-up

- When two backscattered particles hit the detectors or within the detector's response time
- The output is a single signal, proportional to the added energy of the two particles.

- The spectrum loses 2 counts at low energies and gains 1 at high energies.

- This leads to a distortion of the shape of the spectrum.
- Particularly important at high count rates.

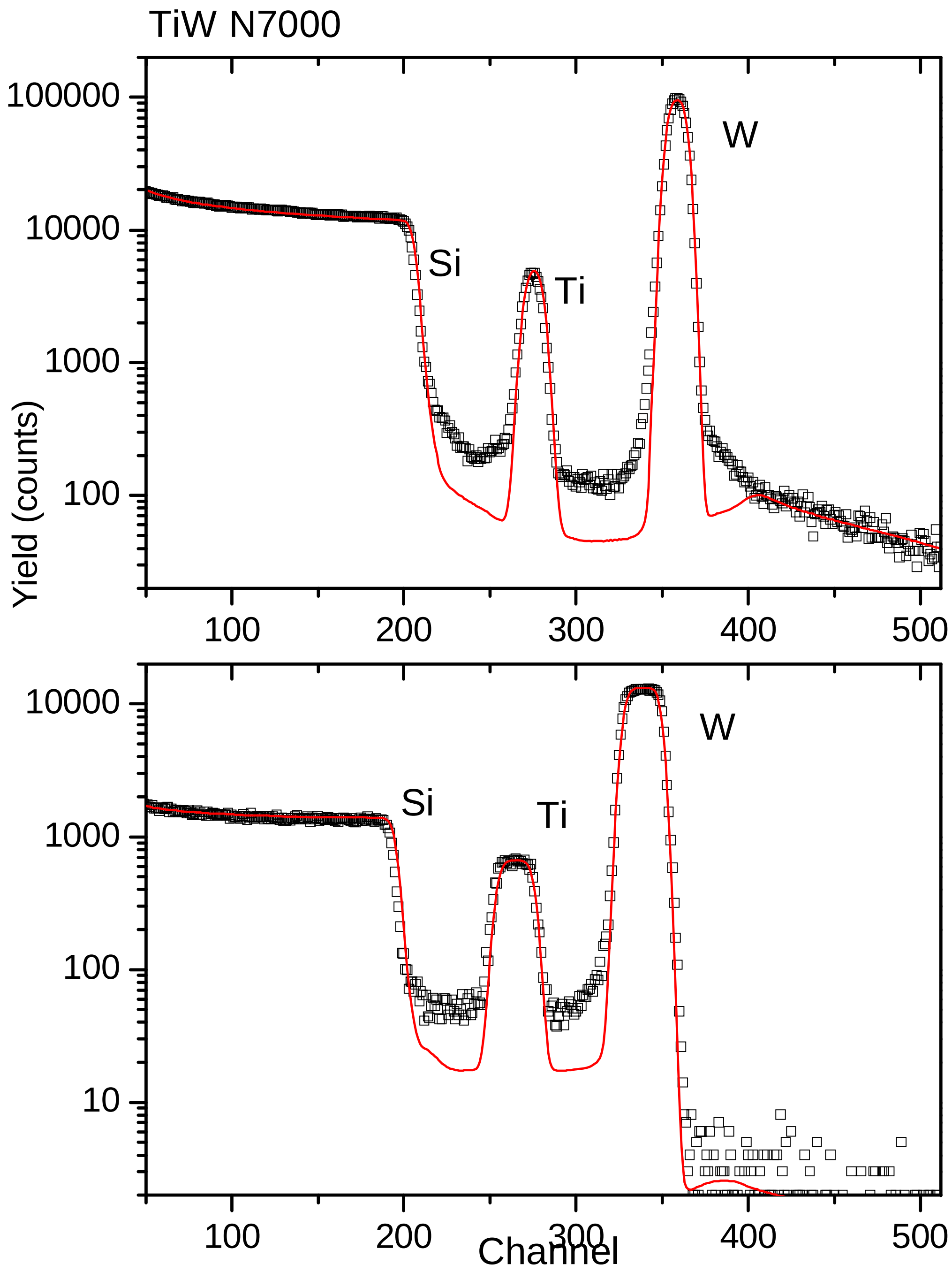
First principles accurate calculation of two- and three-pulse pile-up



Parameters required: livetime; shaping time of amplifier; resolving time of pile-up rejection circuit if present; pulse duration (characteristic of amplifier).

Wielopolski L, Gardner RP. *Nucl. Instrum. Methods.* 1976; **133**: 303. *Nucl. Instrum. Methods.* 1977; **140**: 289. *Nucl. Instrum. Methods.* 1977; **140**: 297.

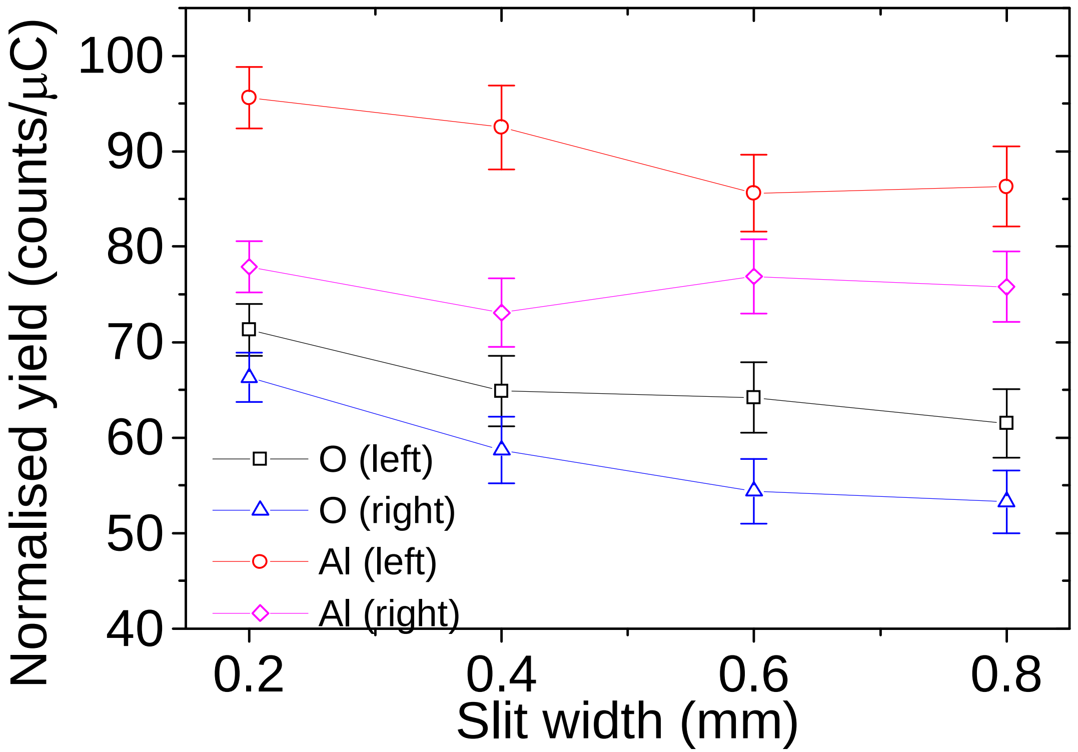
- Two detectors:
  - High count rate
  - Low count rate
- DS not included here



Sources of background

- Slit scattering

Scattering in slits located before sample leads to contamination of beam with lower energy particles ⇒ low energy background



Exists even in systems designed to minimise it
Can only be calculated with full Monte Carlo simulations: not feasible

Sources of background

- Some extra effect not yet understood?

- Claimed by A. Gurbich after a careful experiment in a system without slits, where DS was simulated with Monte Carlo (NIMA 364 (1995) 496)
- Monte Carlo details were not given in paper

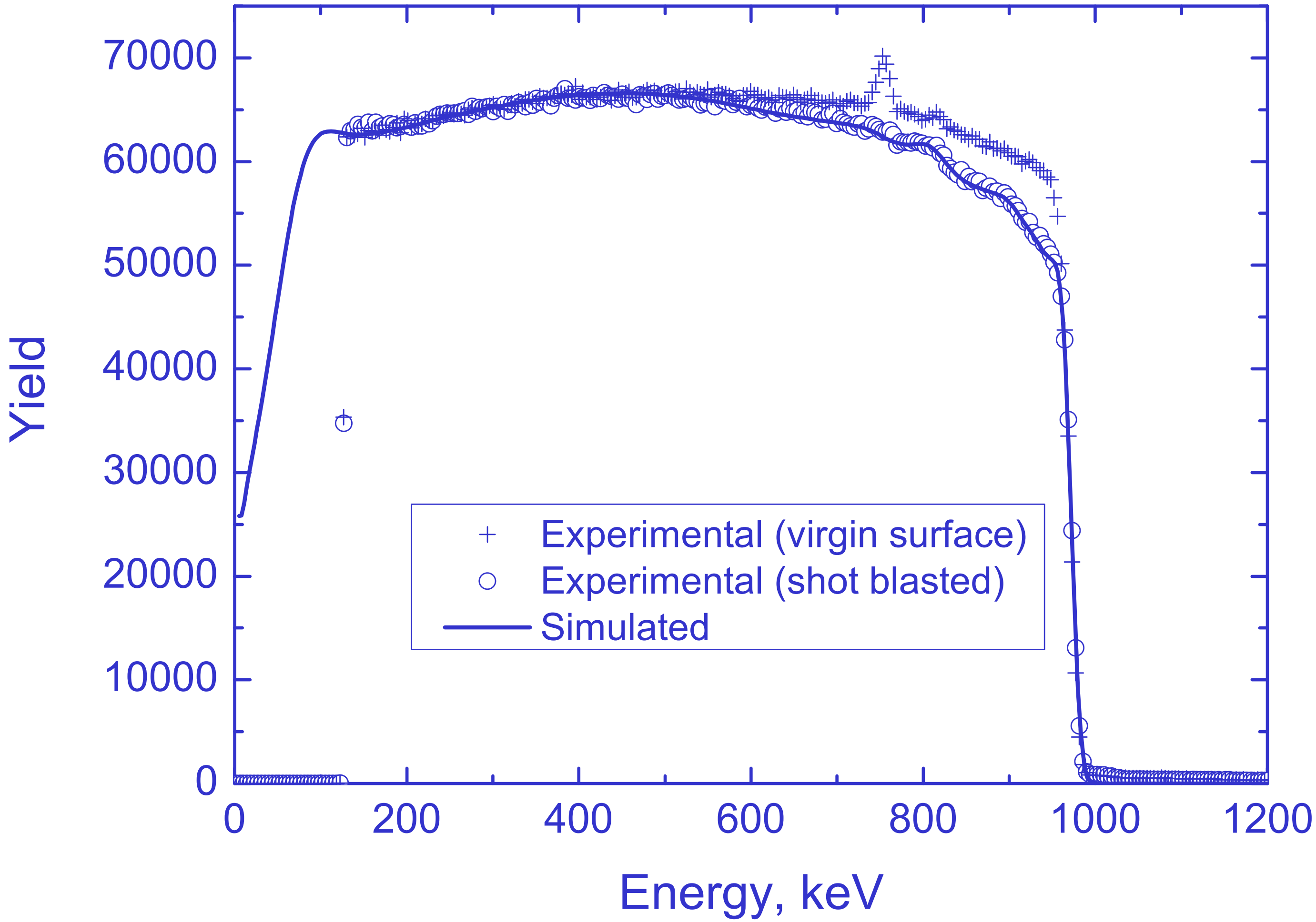
Shape of signals – some effects

- Roughness
- Plural scattering
- Pulse height defect
- Simulation of resonances
- Low energy yield
- Multiple scattering

- Leads to reduced sensitivity to small isolated signals
- Leads to distortion of the signal that must be accounted for in accurate simulations

Shape of signals – some effects

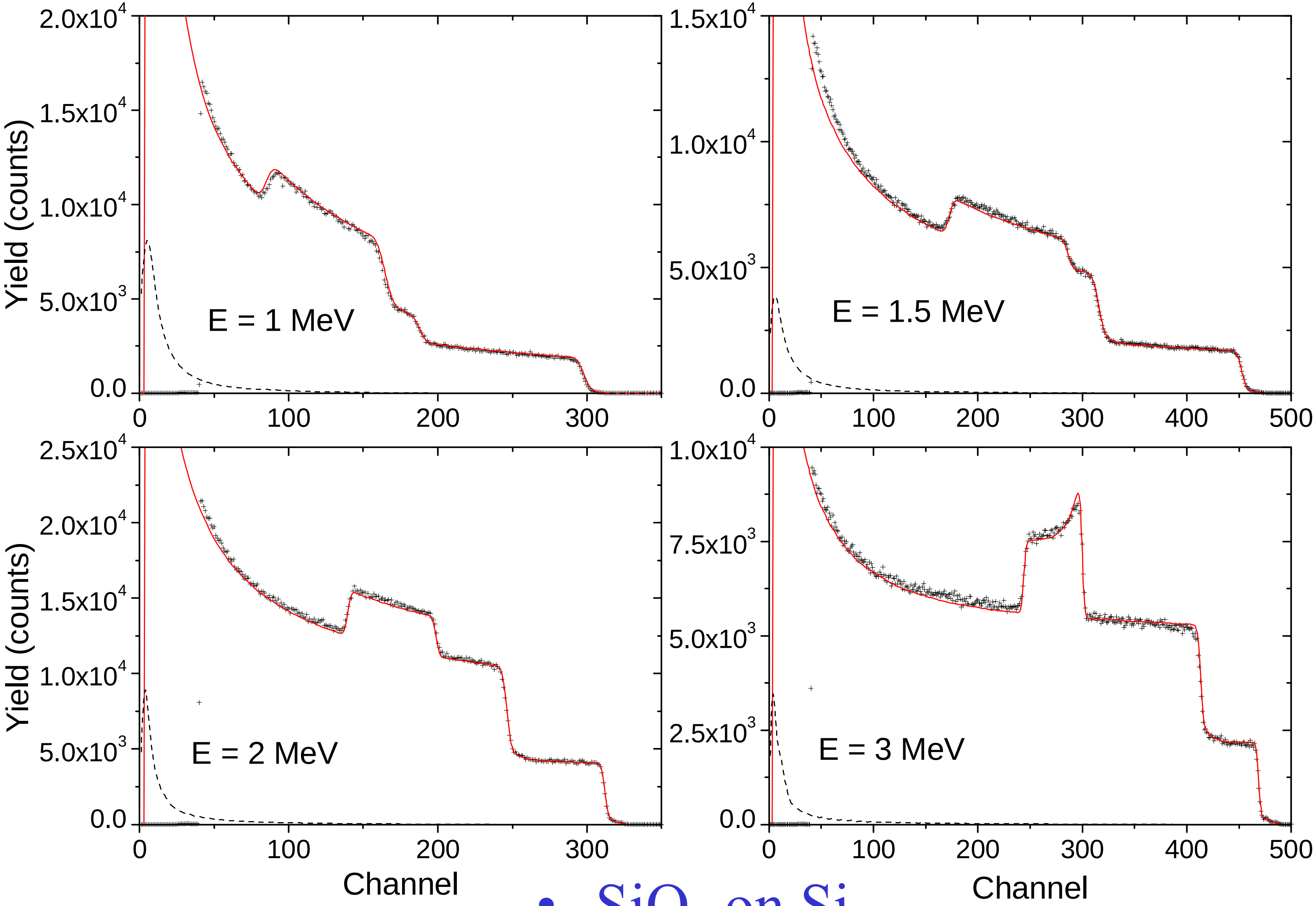
- Roughness



- Model by Molodtsov, Gurbich and Jeynes works well
  - In some cases, perhaps no proper model available

Shape of signals – some effects

- Plural scattering



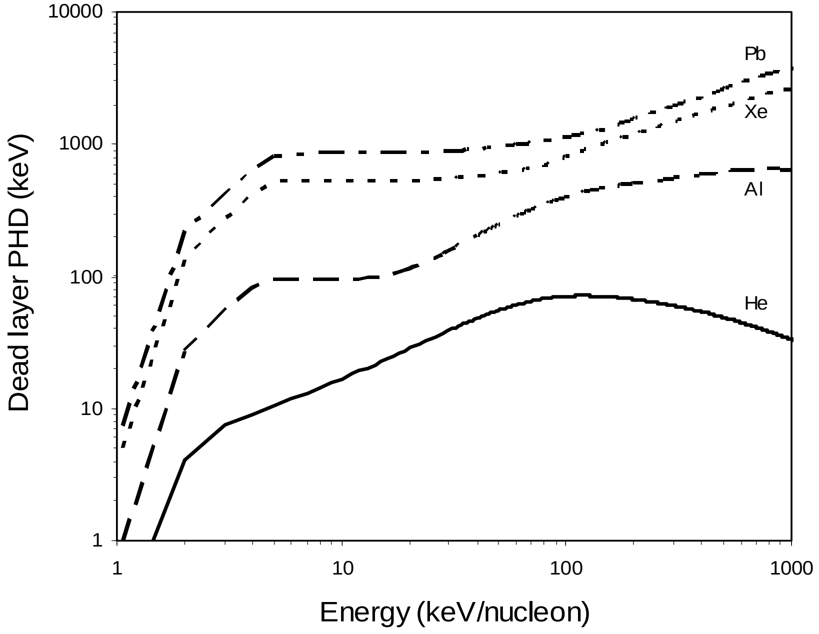
- SiO_2 on Si

Shape of signals – some effects

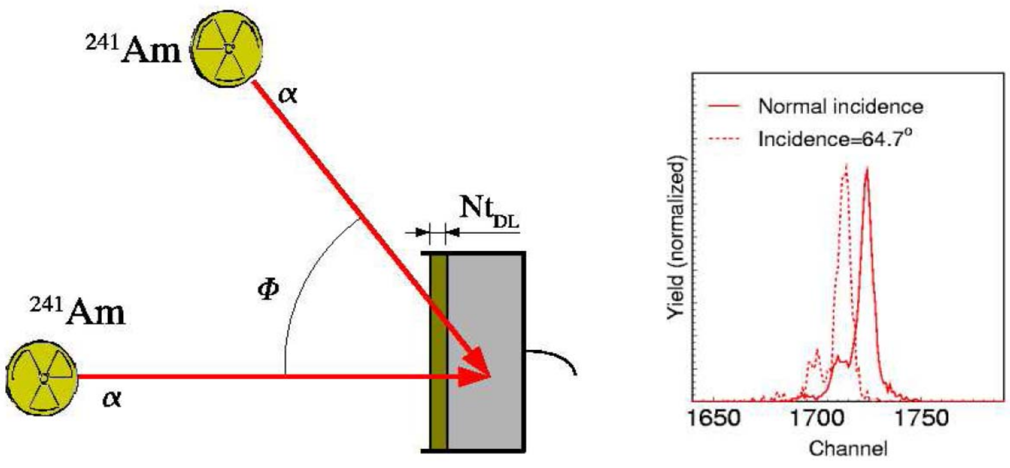
- Pulse height defect

- Si surface barrier detectors have a dead layer where charge is not collected. The detected beam, however, loses energy when crossing it.
- Not all the energy of the beam is transformed in electron-hole pairs, some is lost to non-ionising events. This depends on the beam species and energy.

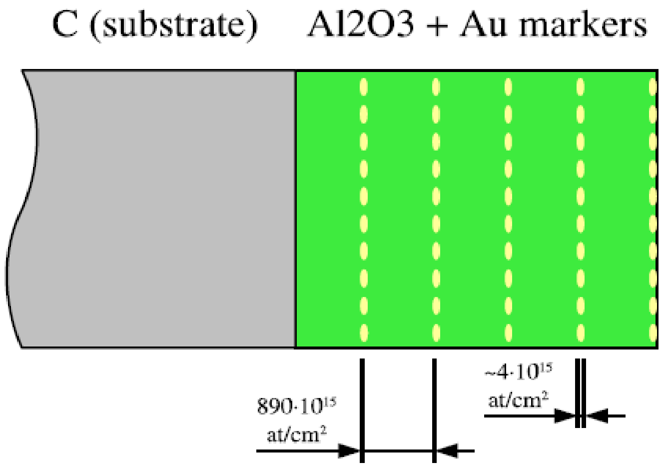
- Energy spectra as measured with a SSB do not exactly represent the energy of the backscattered beam.
- For 4He in Si, this effect can be about 0.5% in yield changes, depending on beam energy.
- For heavy ions, the effect can be much larger.



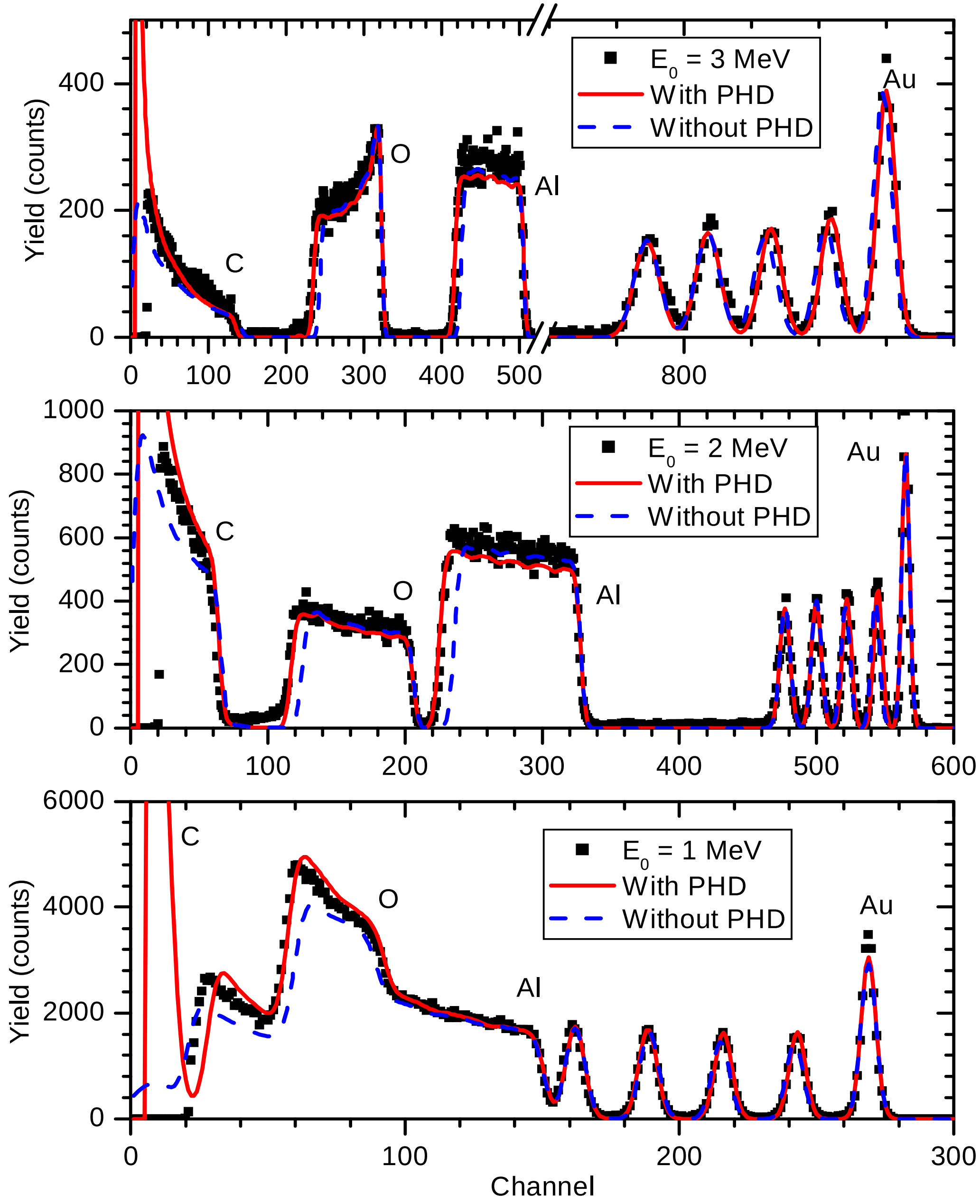
Calculated pulse height defect due to a detector dead layer of 10^{18} Si/cm^2 for four different detected ions



Experimental measurement of the thickness of the detector dead layer



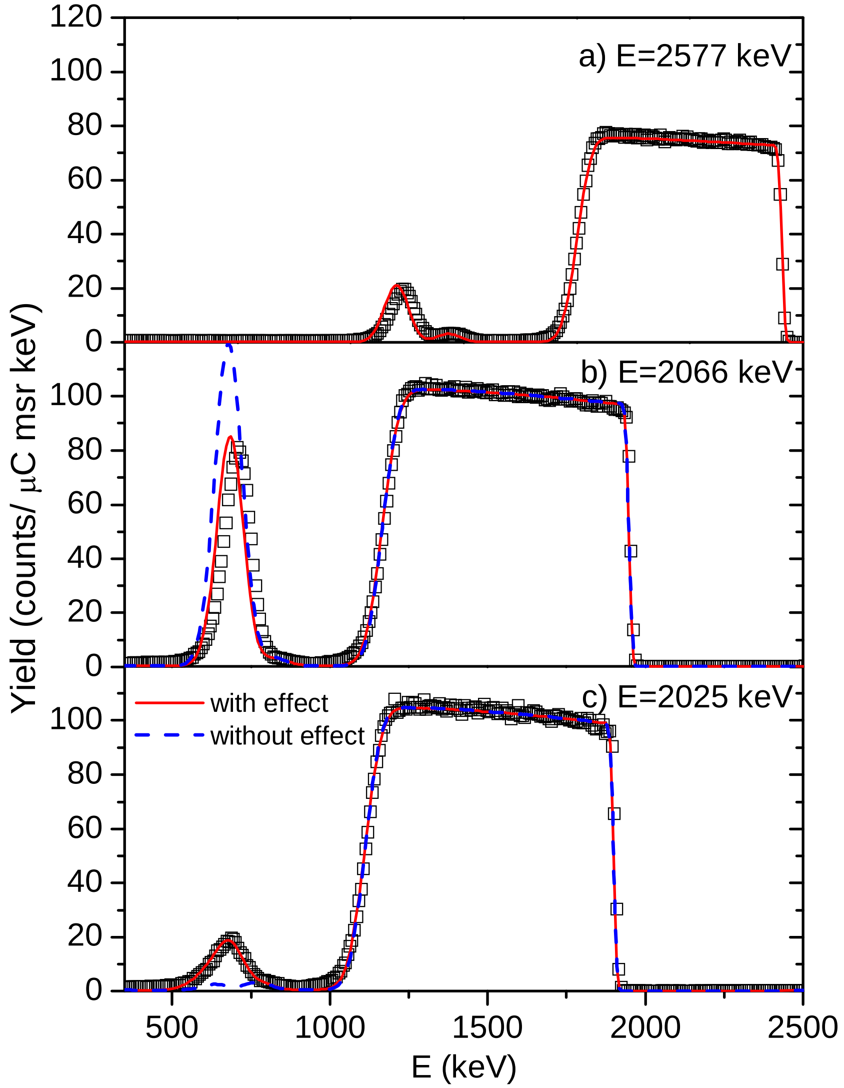
A well-characterised sample consisting of of layers of Au nanocrystals used as markers, embedded in an amorphous Al2O3 matrix deposited on a graphite substrate was measured with different beams: ^{4}He, ^{12}C, ^{16}O, ^{27}Al, ^{28}Si. For each beam, five different beam energies, between 250 and 1250 keV/nucleon, were used.



Experimental RBS data (squares). Simulations considering the PHD correction (solid lines) are compared to simulations that do not take the correction into account (dashed lines). The same energy calibration is enforced for all energies.

Shape of signals – some effects

- Simulation of resonances



- ➢ Energy spread leads to a smearing of the cross section
- ➢ If this is not taken into account, simulated resonances are much sharper than the measured data

Example: Mylar 1 µm /Ni 4.2 µm with p beam

➢ “Double integral”: accurate, hard, slow

“Detailed analysis of the resonant backscattering spectrum for deeply penetrating protons in carbon”
M. Tosaki, S. Ito, N. Maeda, NIMB 168 (2000) 543

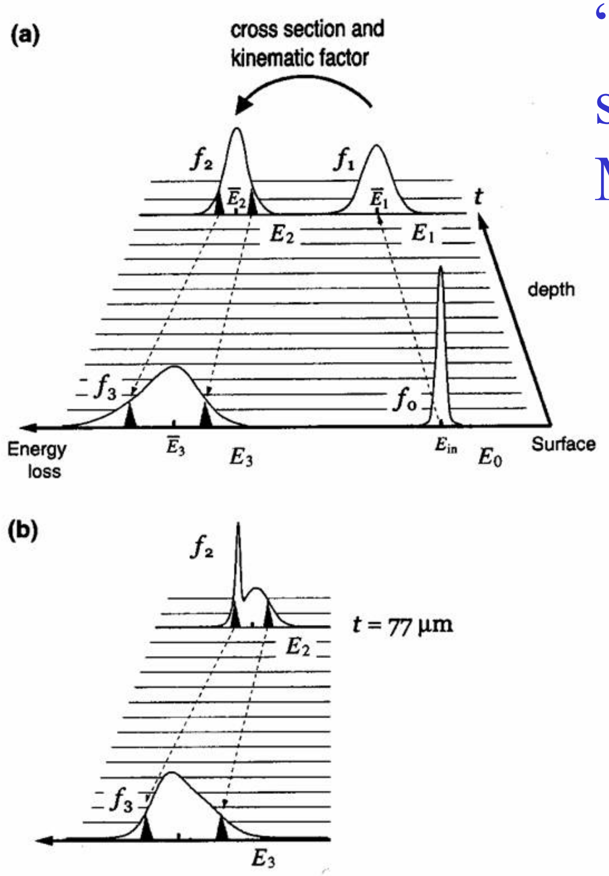


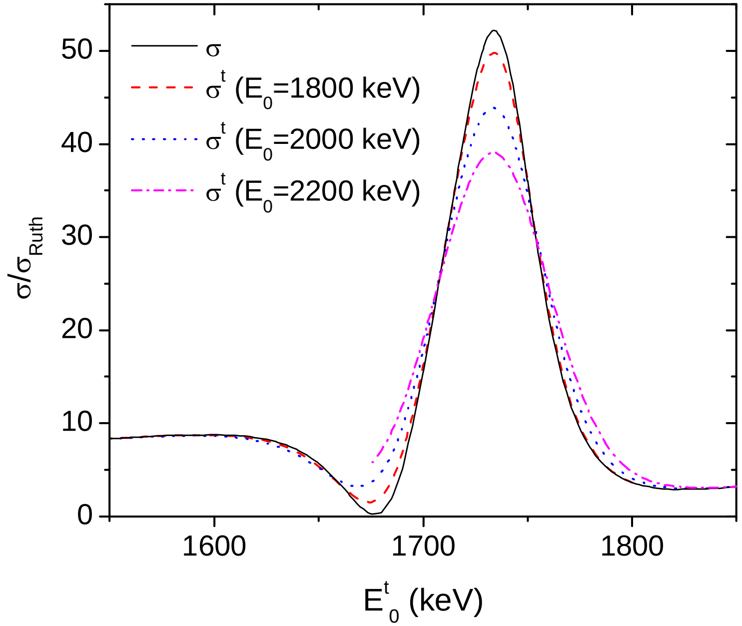
Fig. 3. A schematic illustration of the energy distributions of ions along trajectories in matter: (a) indicates the case in which the normal Rutherford backscattering occurs at a depth t. The effect of energy-dependent stopping power is seen in the behavior of the black patterns indicated in the distributions f_2 and f_3; (b) shows the distributions f_2 at the depth of 77 µm and f_3, particularly for the case of 6.0-MeV proton incidence on the solid carbon target. The distribution f_2 consists of a sharp peak having a ~11-keV width (FWHM) and ~63-keV wide braod part, but the sharp feature is smeared out in the distribution f_3. In this case, the widths for the distributions f_1 and f_3 are found to be 88 and 137 keV, respectively.

Double integral is required:
- on depth of interaction
- on energy before interaction

In practice, for each depth of interaction, ions with different energy must be followed separately, calculating one sub-spectrum for each.

This effect is only important if the cross section changes abruptly, leading to severe distortions of the energy distribution.

➢ NDF: fast, easy, good enough

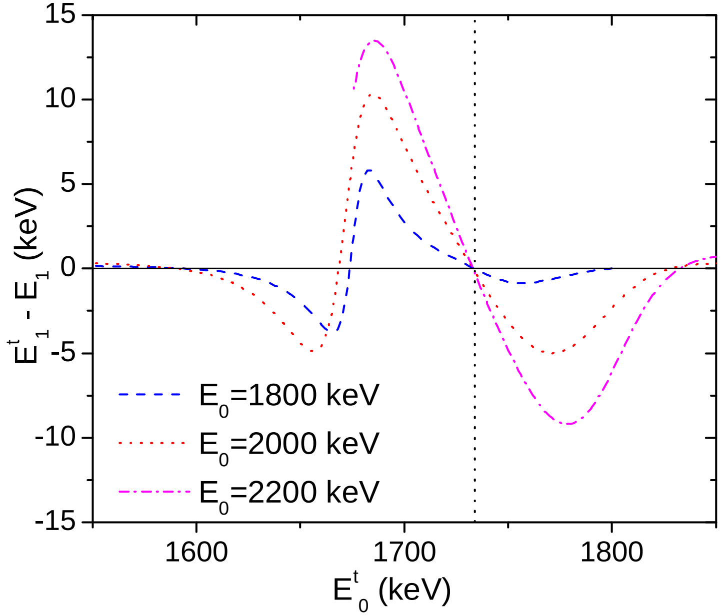


Effective cross section

$$\sigma^t(E^t_0) = \int_{-\infty}^{+\infty} \Gamma^t_0(E - E^t_0, s^t_0)\,\sigma(E)\,dE$$

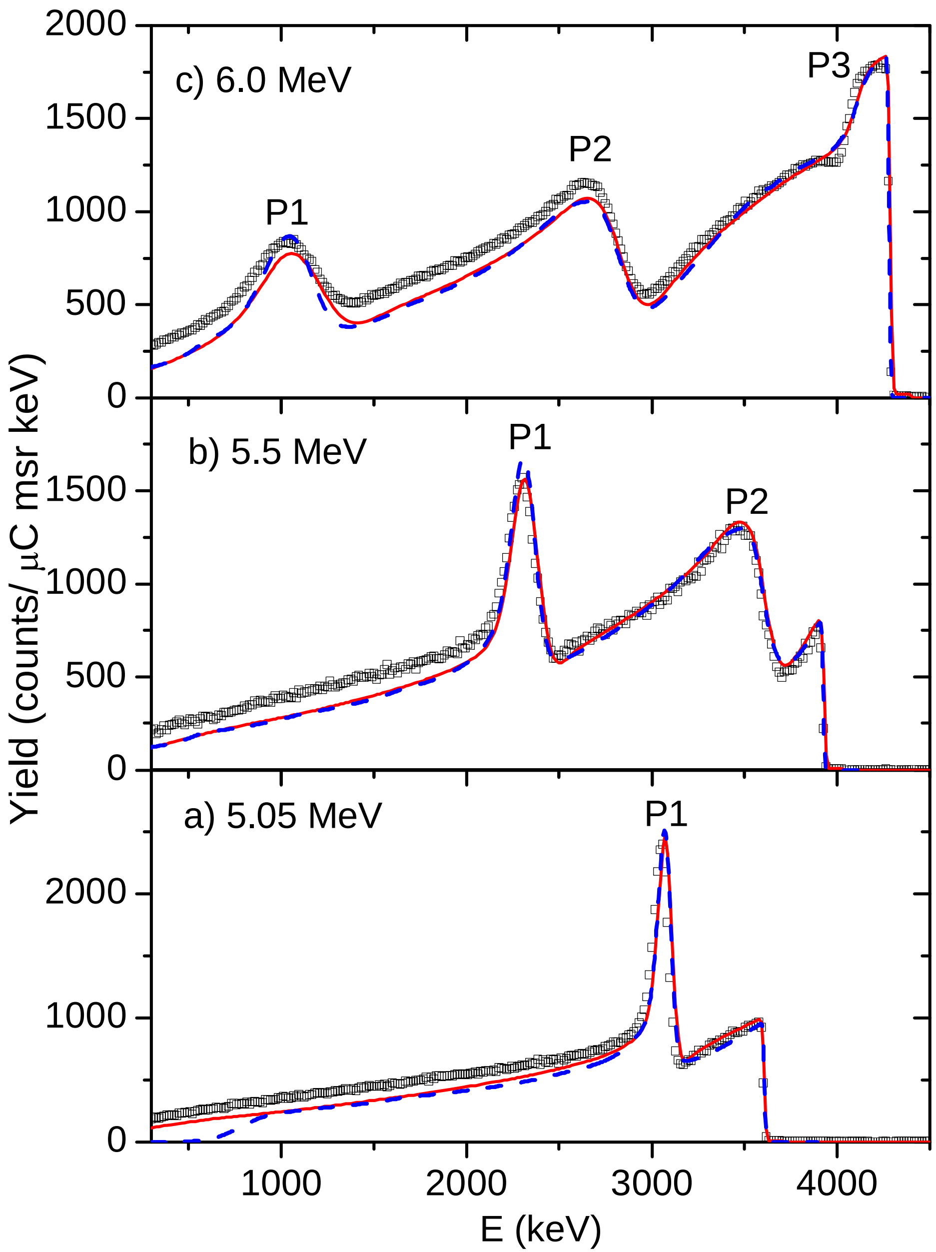
Average energy after interaction

$$E^t_1(E^t_0) = \int_{-\infty}^{+\infty} E_1(E)\,\Gamma^t_0(E - E^t_0, s^t_0)\,\sigma(E)\,dE \Big/ \int_{-\infty}^{+\infty} \Gamma^t_0(E - E^t_0, s^t_0)\,\sigma(E)\,dE$$



➢ Calculations for protons in C

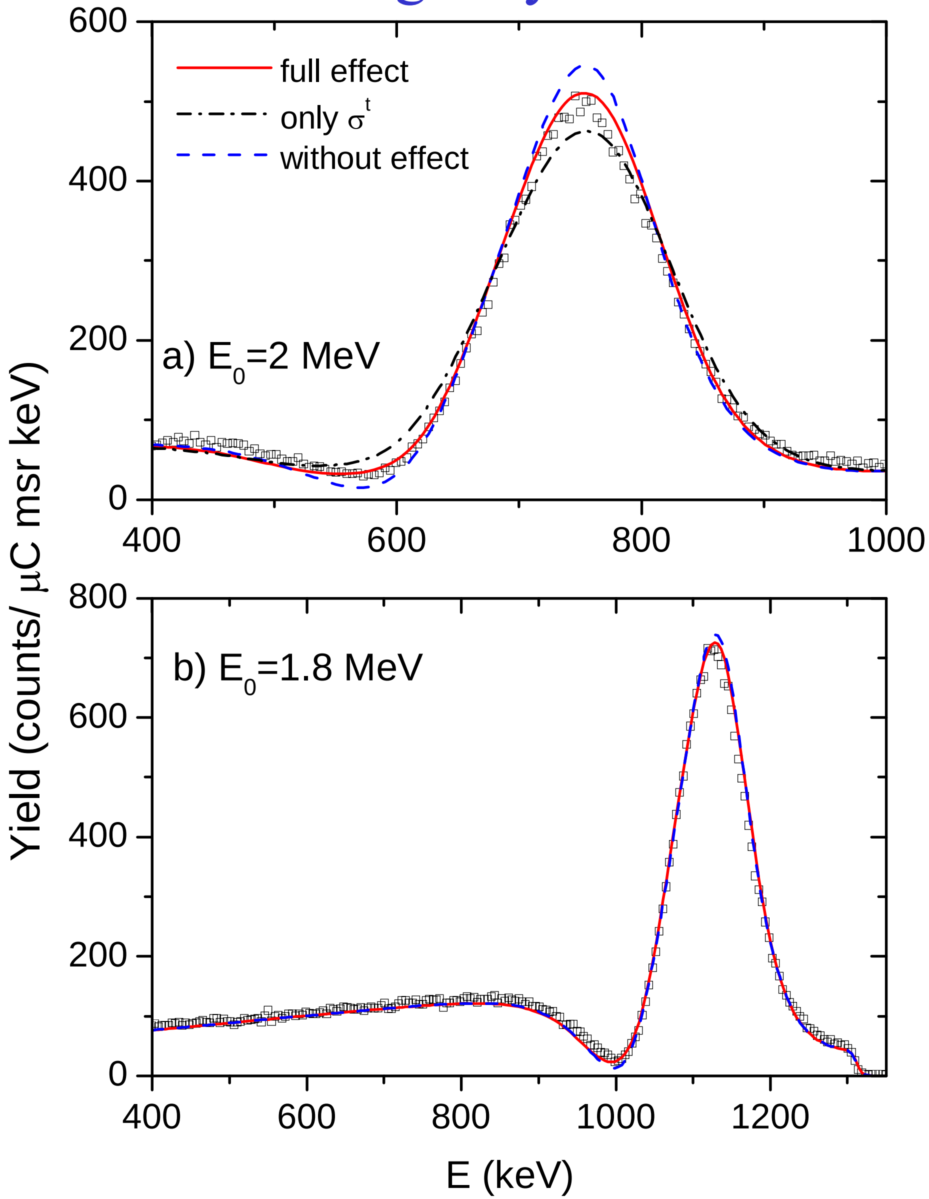
➢ Comparison between NDF and full model by Tosaki



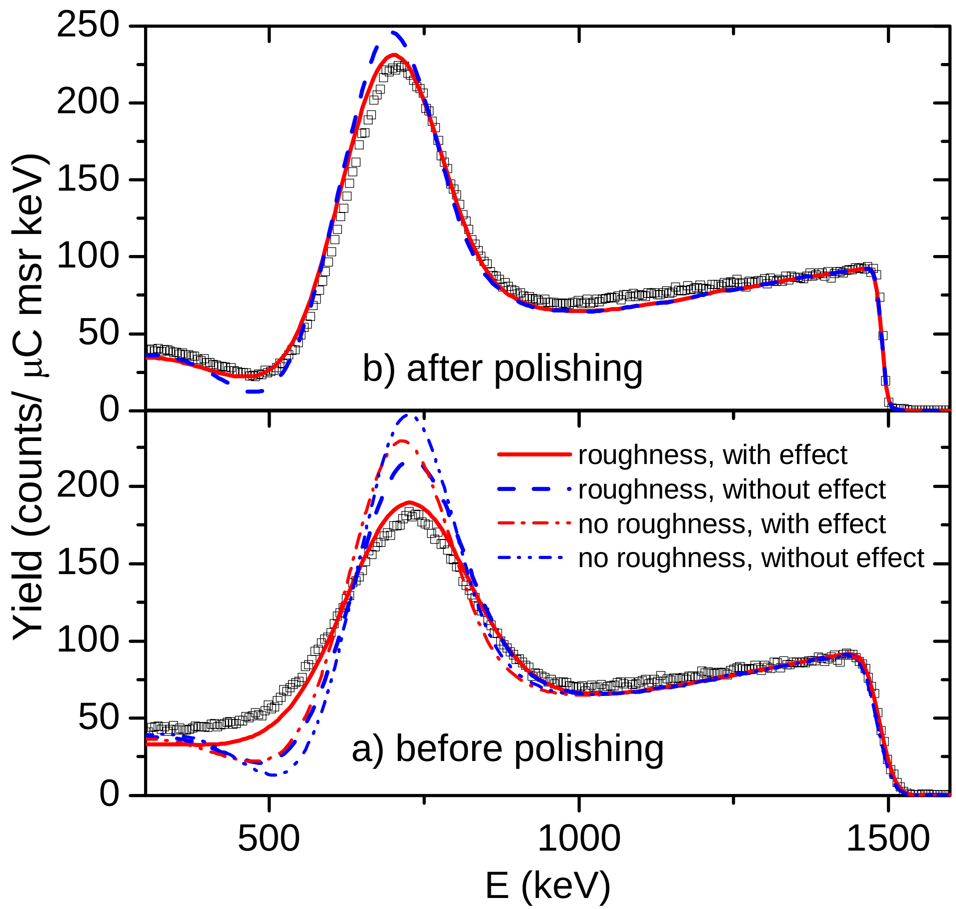
➢ Full model does not include Tschälär effect on straggling

➢ Comparison with data: protons on C

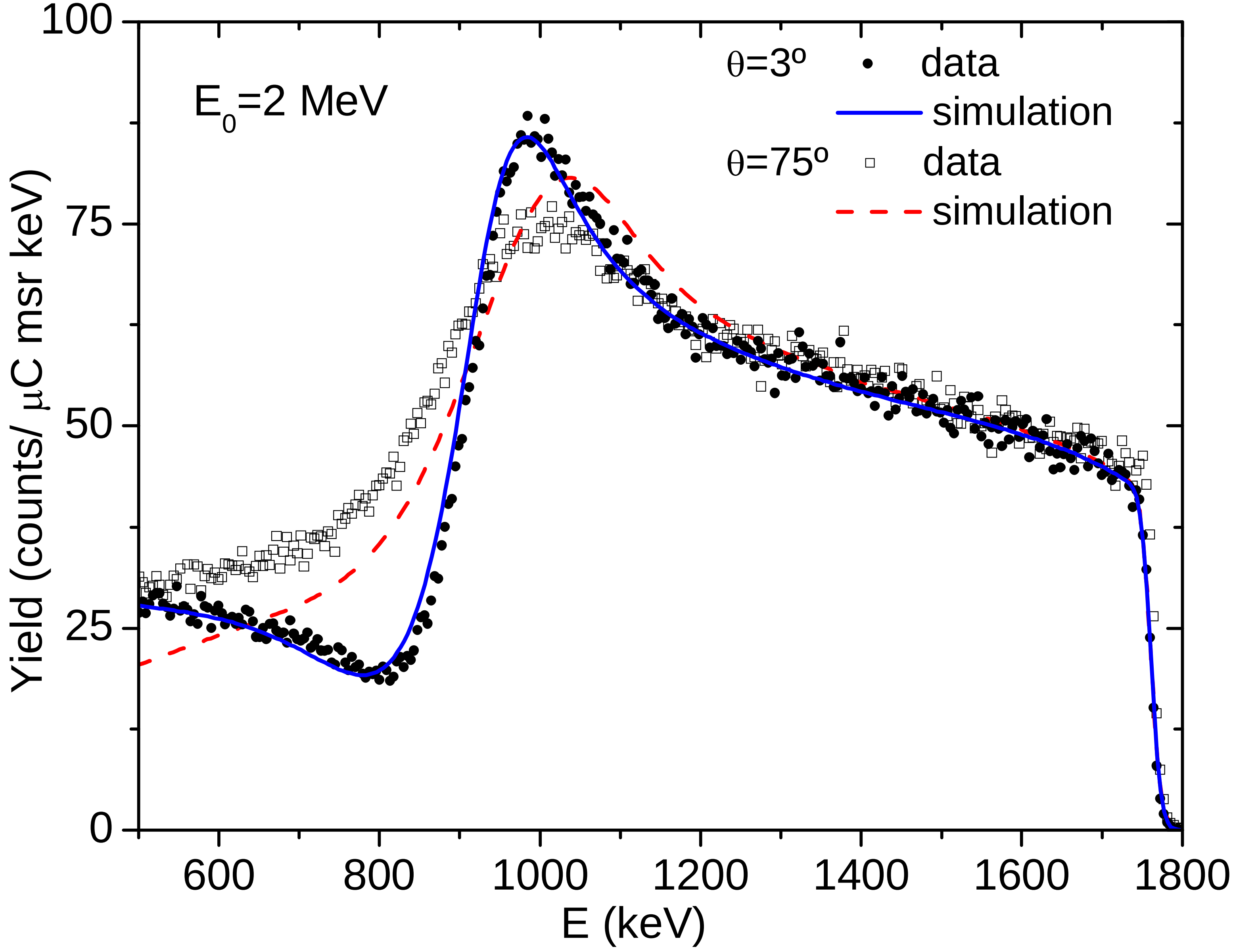
➢ glassy C



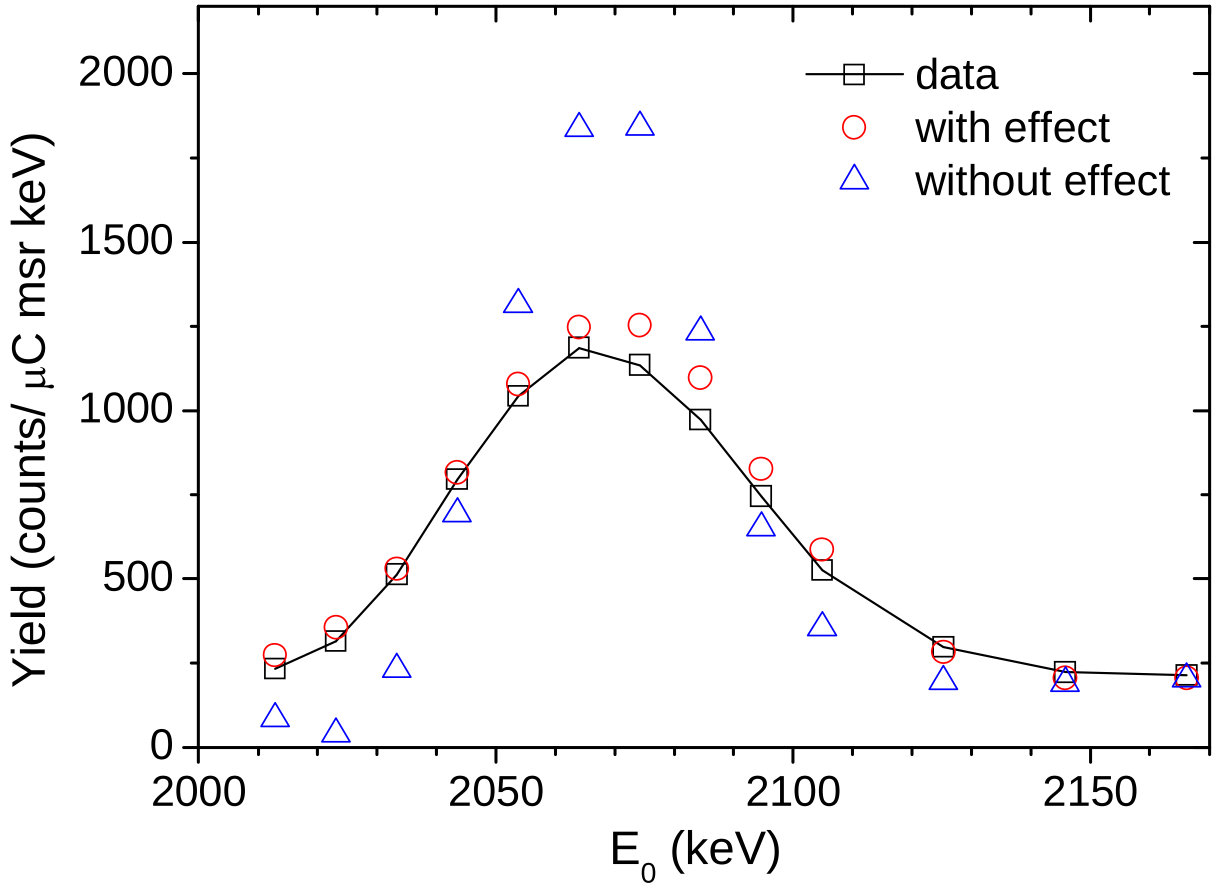
➢ Pyrolytic graphite



➢ Where the model fails: grazing incidence



➢ 1 μm Mylar film under a 4.2 μm Ni film



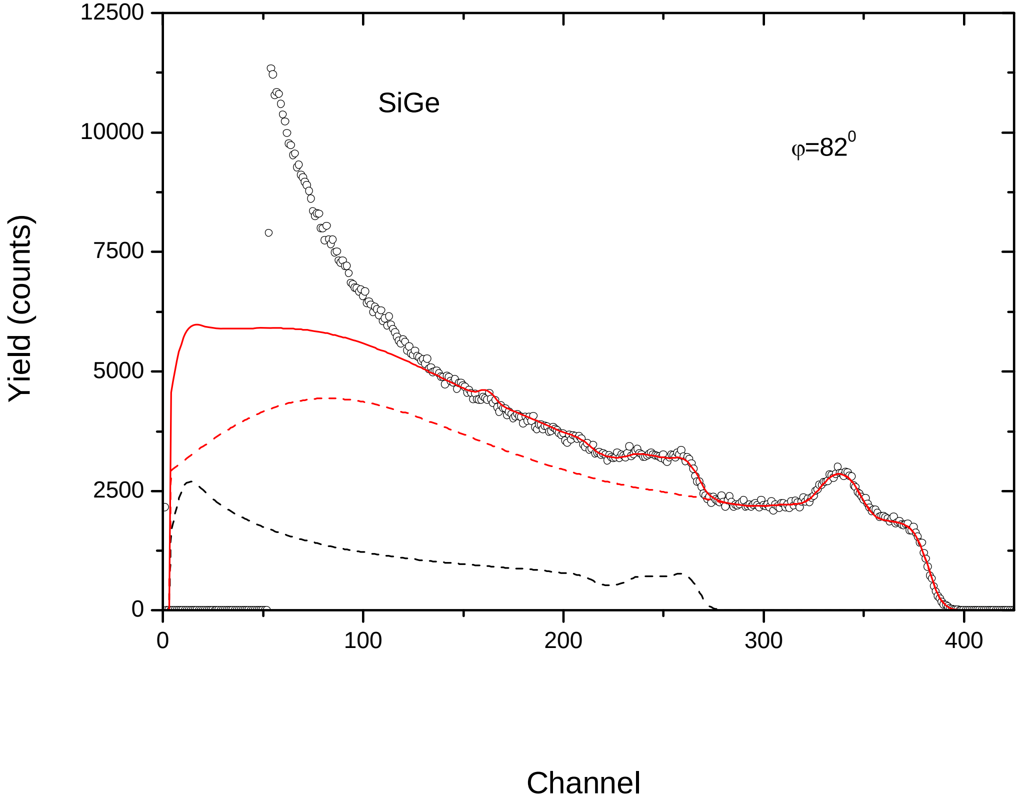
- ➢ Total yield of films affected
  - ➢ Factor of 10 in worst case scenario!!!
  - ➢ 30% error at yield maximum

Shape of signals – some effects

- Low energy yield

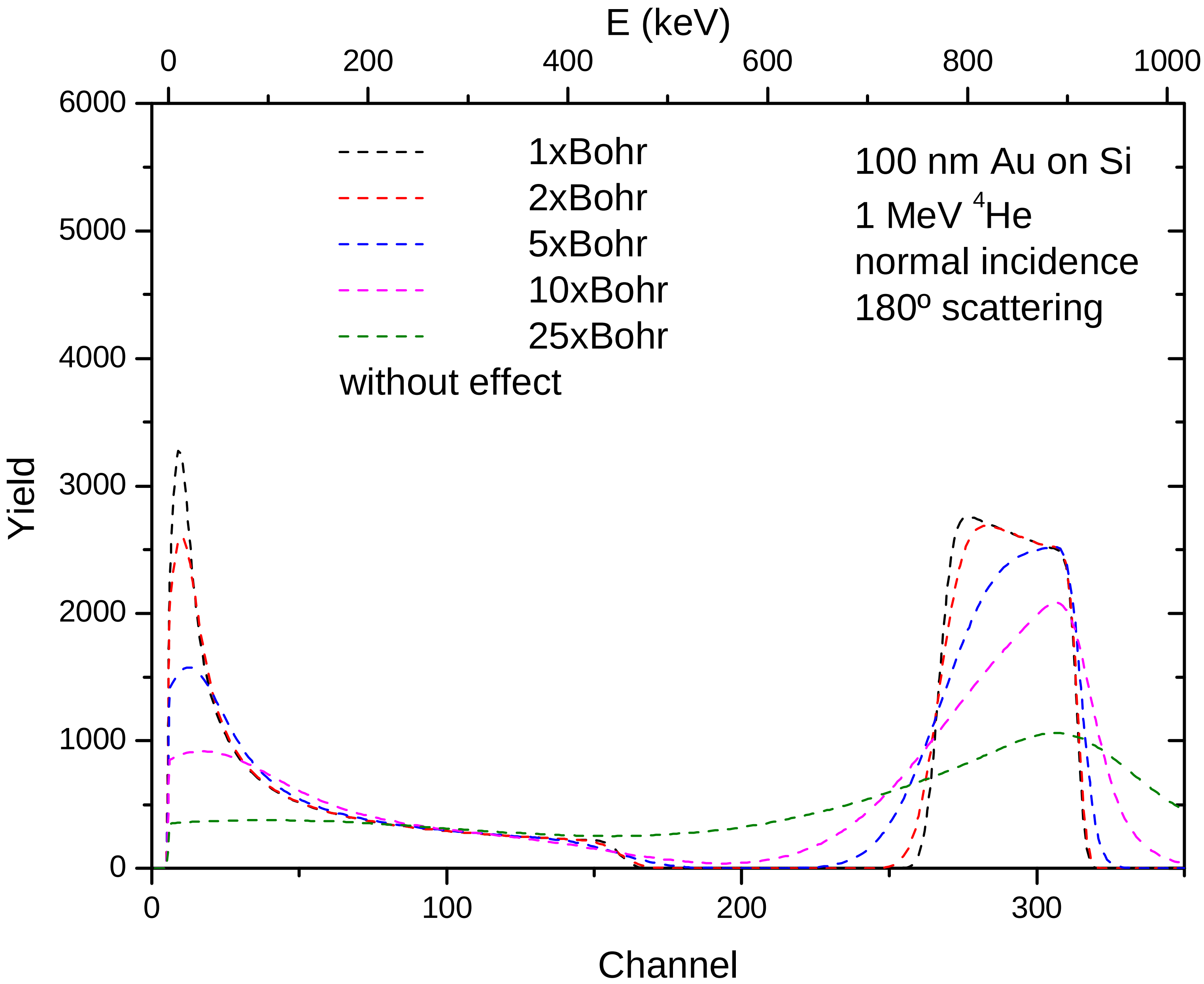
➢ At low energies, simulations drop while data increases

➢ Counts are lost in the simulation due to energy spread; tails of the calculated energy distribution functions are at negative energies (!)

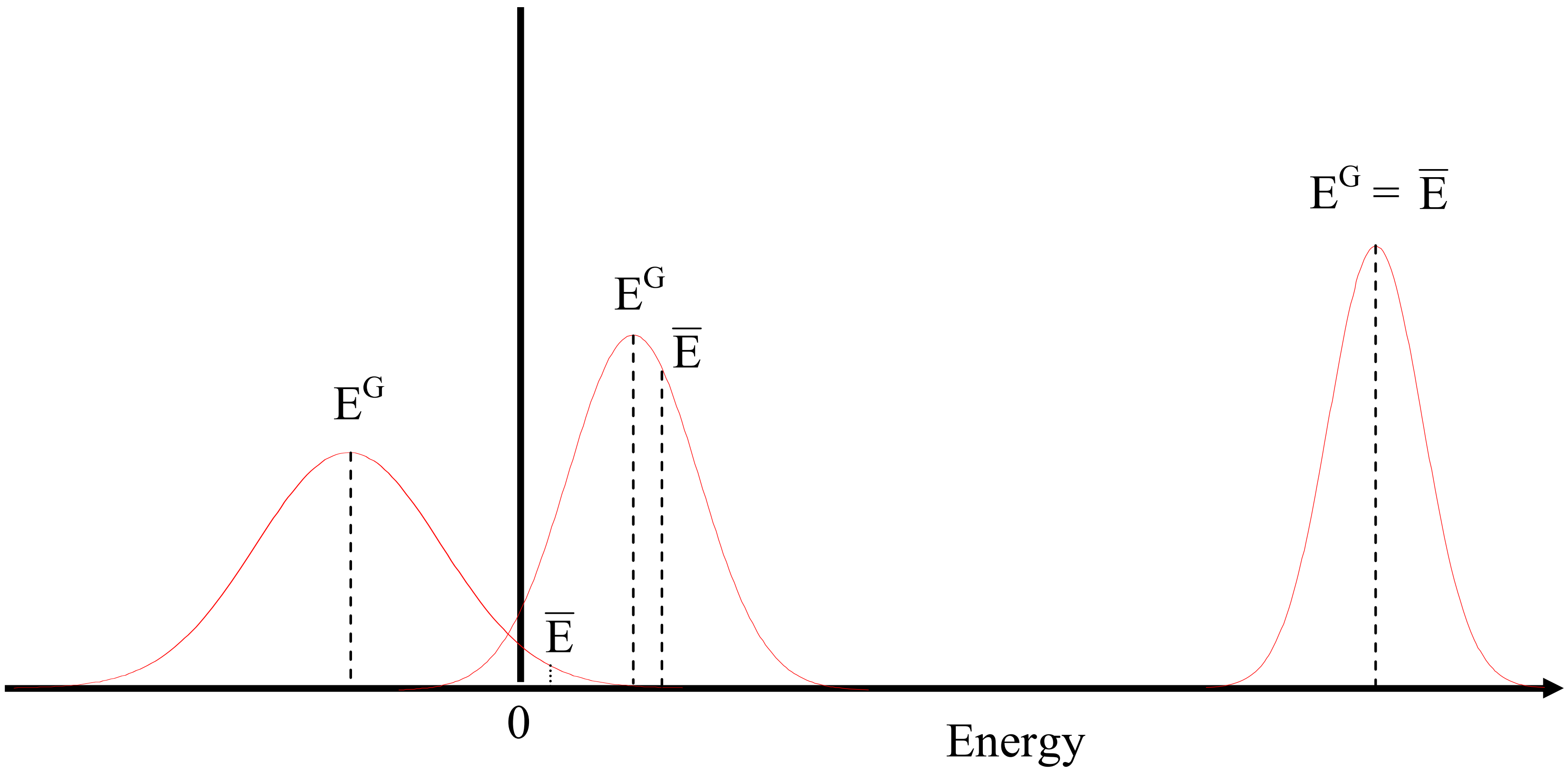


➢ "This problem probably cannot be solved" (Edit Szilágyi, IBA2005)

Low energy yield

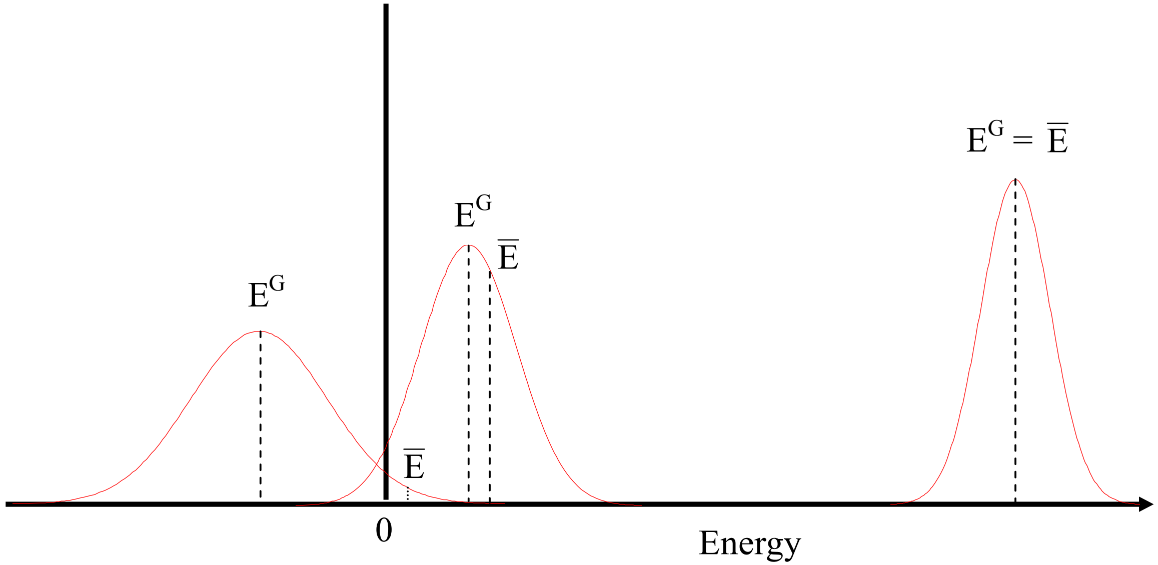


➢ What is happening?



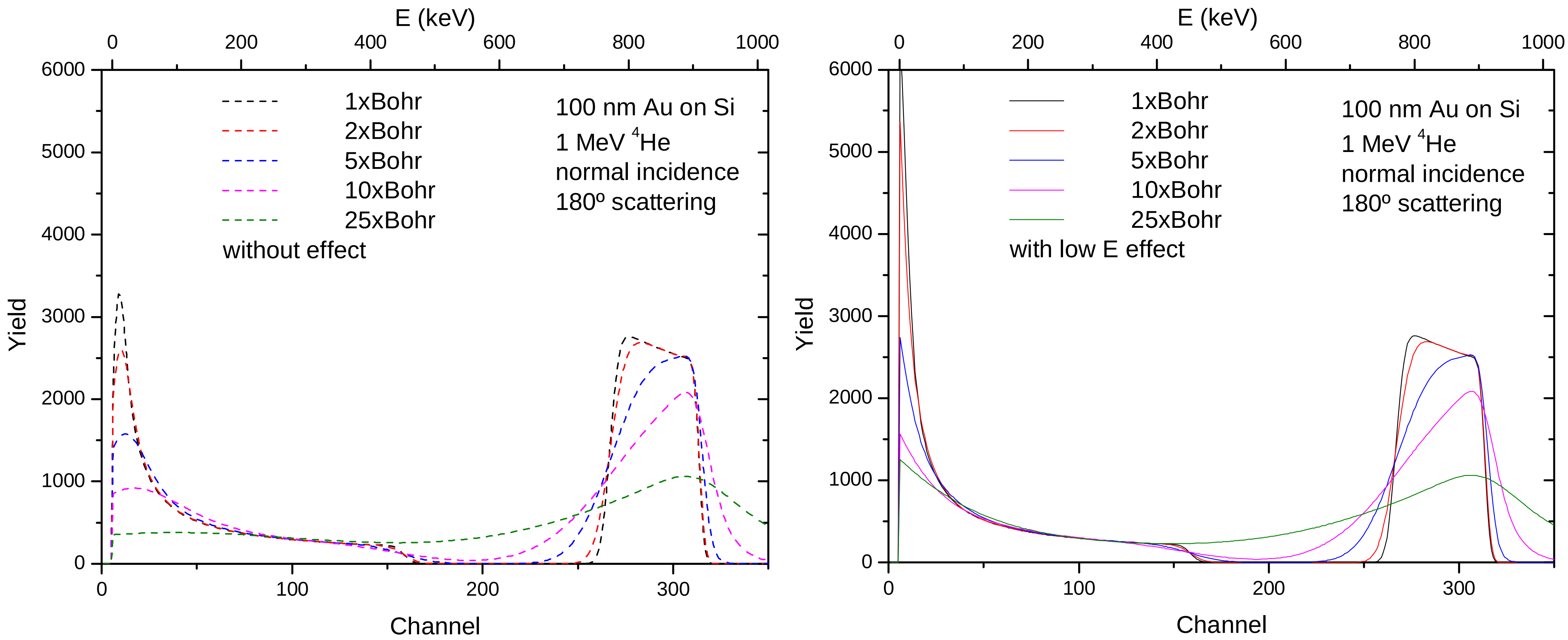
- Most codes stop the calculation at channel 0, not energy 0.
- At $E^G<0$, particles in the positive branch of the Gaussian are discarded

➢ NDF model



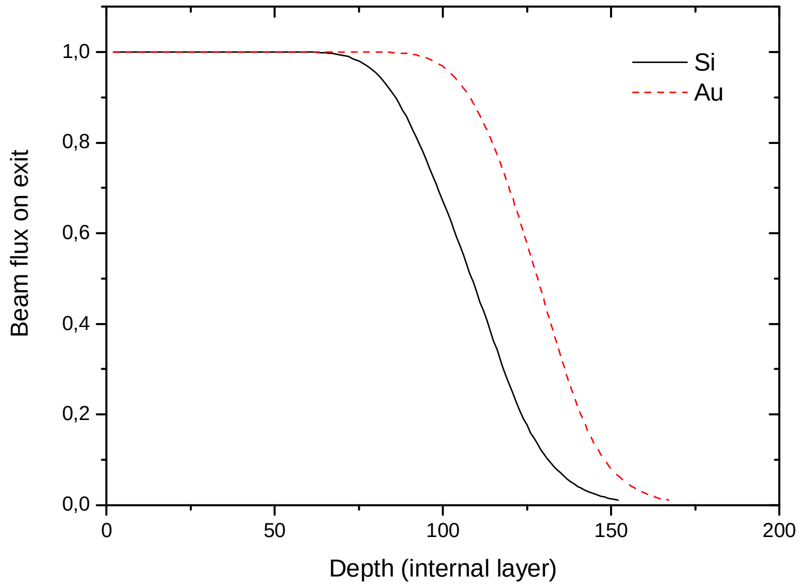
- NDF goes to energy 0 (which leads to virtual negative channels).
- NDF follows the Gaussian as long as 1% of it remains positive
- The Gaussian is no longer the energy distribution of the beam. Its positive part is. The Gaussian keeps a role as a convenient mathematical construct.
- Physical quantities are calculated for the average E, not E^G (or integrated on E).

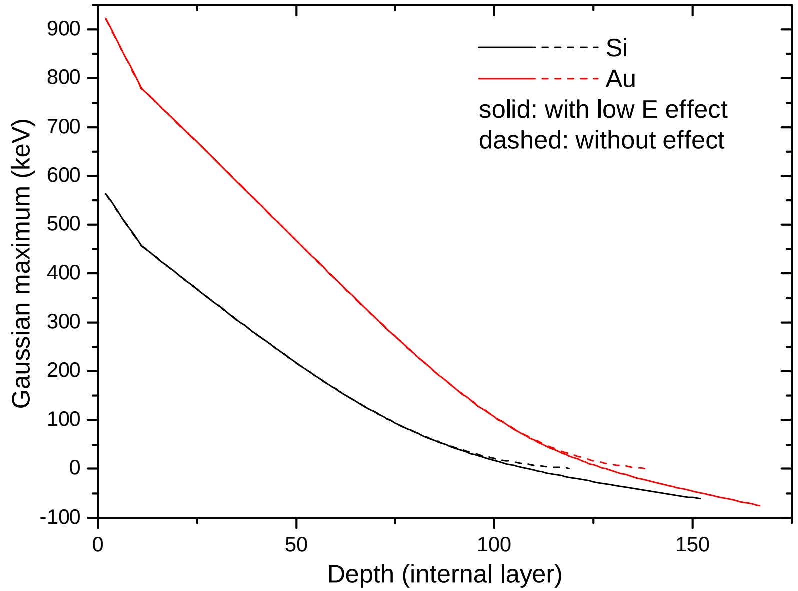
➢ Some results

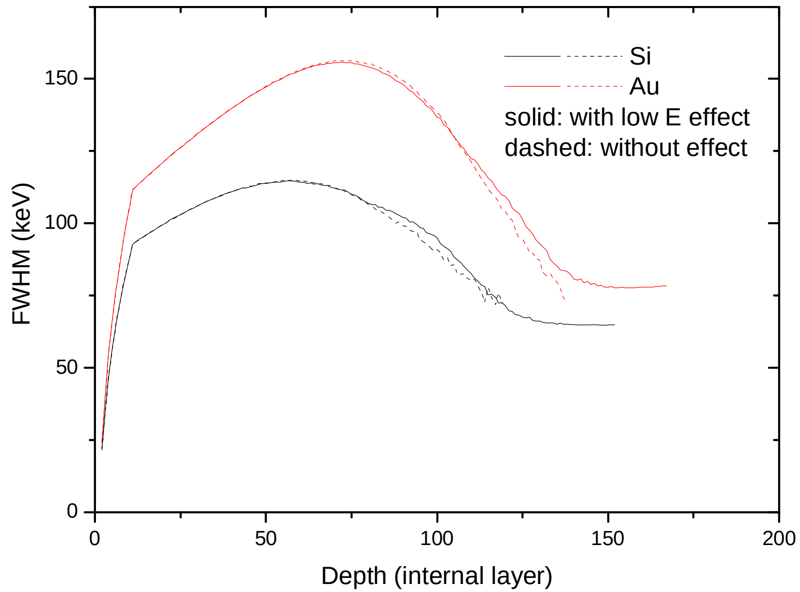


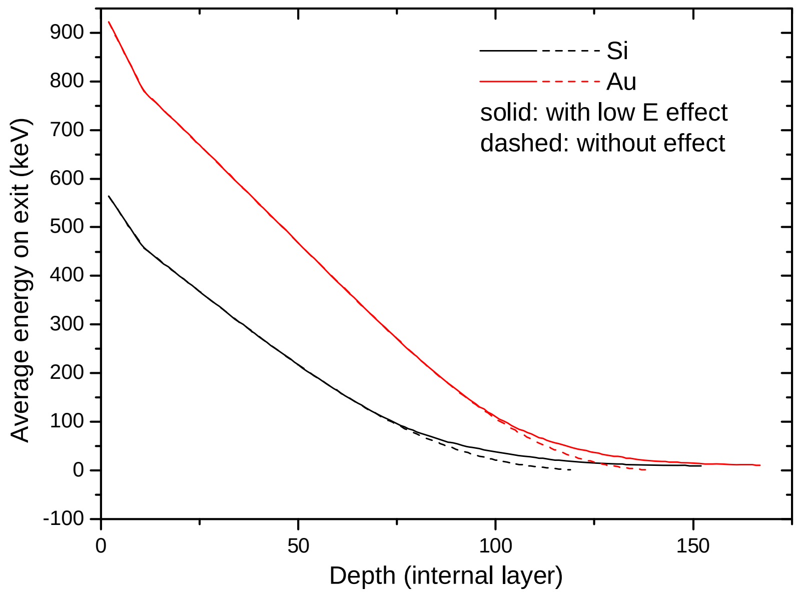
➢ Differences only below 50 keV

➢ Details of the 5xBohr calculation

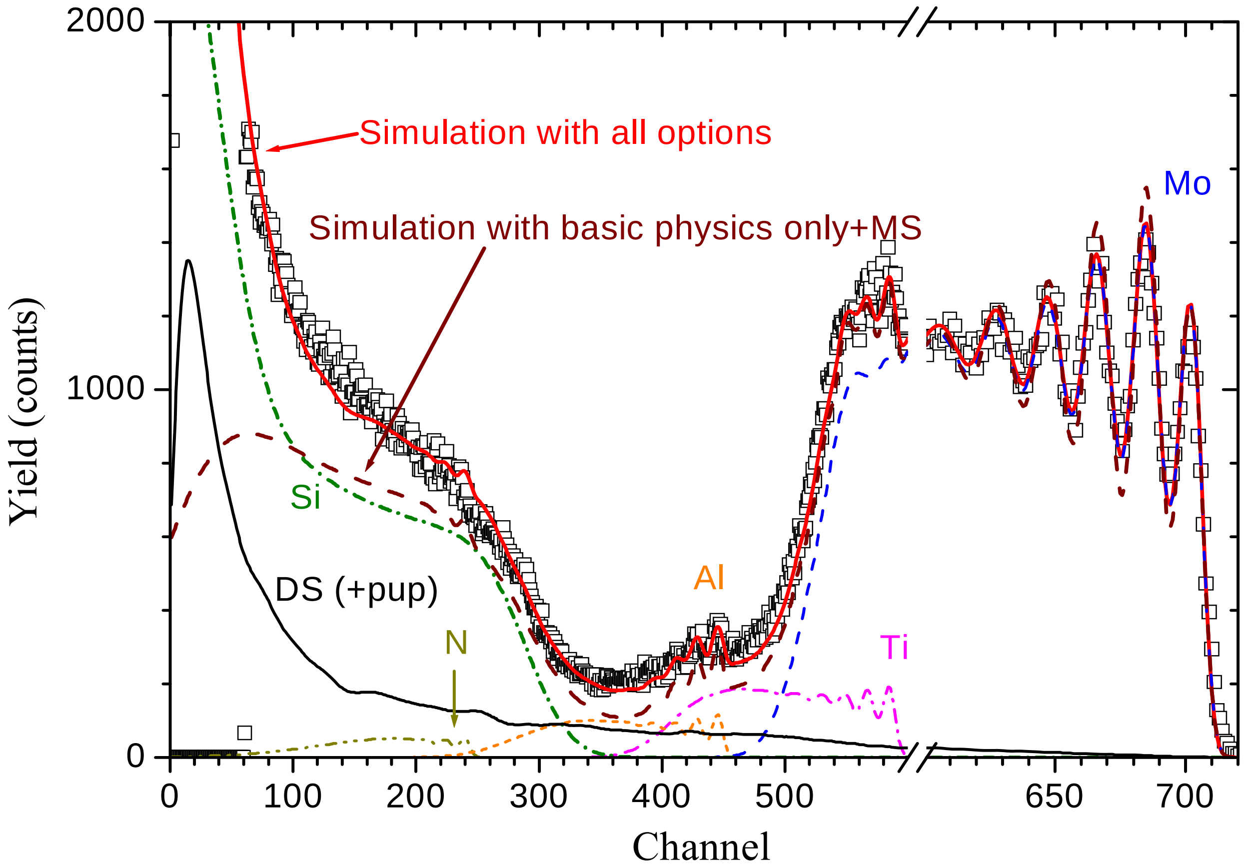








Pure simulation of grazing angle RBS: 5º in Cornell geometry



Advanced physics included

- ✓ Roughness (as given by AFM)
- ✓ Double scattering at grazing angle
- ✓ Realistic pulse pile-up
- ✓ Low energy yield:
  - ✓ Energy distribution of beam is followed untill all ions are at rest
  - ✓ Energy 0, and not channel 0, is considered (implies using virtual negative channels that still lead to yield at positive channels)
- ✓ All contributions to energy spread via DEPTH code

RBS spectrum of a Si/(Ti0.4Al0.6N 25.2Å /Mo 14.9Å)×10 multilayer measured at 5º grazing angle. A full simulation including double scattering (DS), pulse pileup (pup), roughness and an improved low energy yield calculation is shown. The calculated partial signals of the elements are shown. A simulation including only basic physics (but with the correct energy straggling) is also shown for comparison.

Multiple scattering – some effects

- Energy spread
- Effect of scattering angle spread
- Effect of pathlength spread

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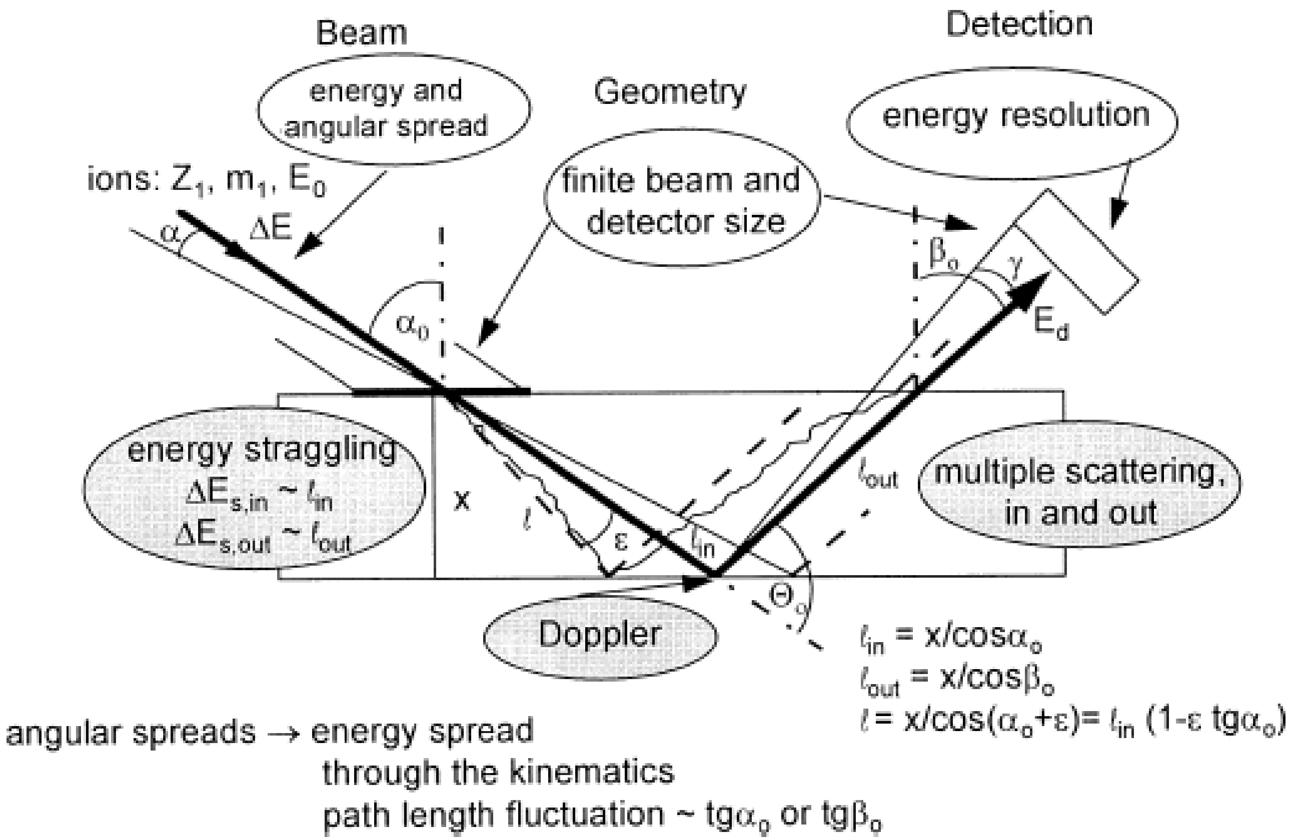
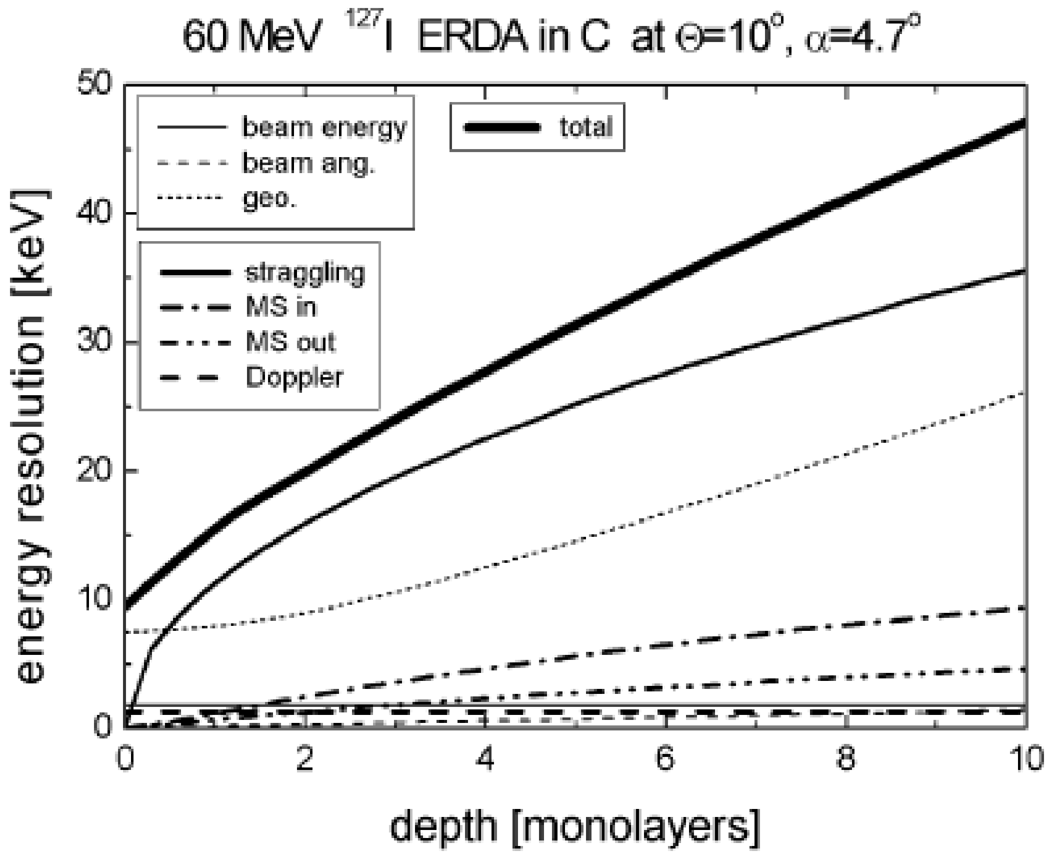


Multiple scattering – some effects

- Energy spread

- In some situations, multiple scattering is the dominating contribution to energy spread
  - Grazing angle
  - Heavy ions
  - Low energies



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Multiple scattering – some effects

- Scattering angle spread
  - Spread of scattering cross section
  - Spread of kinematic factor
- Pathlength spread
  - Spread of scattering centers on way in
  - Spread of energy lost on way in
  - Spread of energy lost on way out

- Shape of signal and total yield change
- Analytic calculations require very strong approximations
- In practice, some signal features are never well simulated

- Monte Carlo may be the only solution, but it has its own problems

Conclusions

- Correct use of software requires knowing the phenomena that influence the data.
- Some effects are still not well simulated.
- Software does not replace the judgment of the analyst.