PIGE Codes Meeting: ERYA-Profiling

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Index

Introduction

- **During the presentation the following conventions are issued.**

$k = \xi / \epsilon_{MAX}$ Landau k-factor

$\xi = \frac{2.5507 * 10^{-7} Z M n}{A \beta^2} [keV]$ Average Energy Loss

$\epsilon_{MAX} = \frac{2 m_e \beta^2 \gamma^2}{1 + 2\gamma \frac{m_e}{m_p}} [keV]$ Maximum transferable energy from a single collision

$\beta = \frac{\sqrt{2 m_p E + E^2}}{m + E}; \gamma = \frac{1}{\sqrt{1 - \beta^2}}; m_e = 511\, keV; m_p = 938272\, keV$ Relativistic parameters

$\lambda = \frac{\Delta}{\xi} - 1 + \gamma_{EM} - \beta^2 - \ln(k)$ Landau λ variable

$\Delta = \overline{\Delta E} - \Delta E$ Difference between average energy relative to the distribution and energy loss

Ω Detector Resolution and Doppler Broadening Variance

Yield Calculation on ERYA-Profiling

- **ERYA-Profiling performs the numerical calculation of the yield by multi-variable numerical integration in terms of energy related to the convolution of distributions:**

$$Y(E_0)=4\pi\varepsilon_{\text{abs}}(E_\gamma).N_p.N_{av}.A^{-1}\int_0^{E_0} Z(E).f_m(E).f_i(E)/S_m(E)\,dE \quad [1]$$

$$Z(E)=\int_{-\infty}^{\infty}\int_{-\infty}^{+\infty}\sigma(E-E')f_S(E'')f_D(E''-E')\,dE'dE'' \quad [2]$$

- **However the following assumptions are applied to simplify the evaluation:**
  - For each layer, the stopping-power, atomic and isotopic fraction are assumed constants, converting equation (1) to a sum (3) where the energy of the beam (E) are treated as a formal constant with an average value. $\overline{E}_k$
  - The cross-section evaluation depends from the double integral convolution (2) from the different distributions in function of energy (E' and E")

$$Y(E_0)=\sum_{k=1}^{n} Y_k(\overline{E_k}),\text{where} \quad Y_k(\overline{E_k})=4\pi\epsilon_{\text{abs}}(E_\gamma)N_{av}N_p f_{mk} f_i A^{-1}(\Delta E)_k S^{-1}(\overline{E_k})Z(E) \quad [3]$$

Convolution Formula on ERYA-Profiling

- The Distributions Convolution with the Cross-Section are evaluated directly by a numerical double integral, using the following formula:

$$\sigma\left(\overline{E_k}\right)=\frac{\int_{-3\Omega+\lambda_0}^{3\Omega+\lambda_{0,995}}\int_{-3\Omega+\lambda_0}^{3\Omega+\lambda_{0.995}} F_T(x)\,F_S(y-x)\,\sigma\left(\overline{E_k}-y\right)dx\,dy}{\int_{-3\Omega+\lambda_0}^{3\Omega+\lambda_{0.995}}\int_{-3\Omega+\lambda_0}^{3\Omega+\lambda_{0.995}} F_T(x)\,F_S(y-x)\,dx\,dy} \quad [4]$$

- The integration domain are truncated to 3-sigma for the Gaussian type Doppler/Resolution (F_T) distribution, and 99.5% of statistical significance for the Straggling (F_S) distribution for which we will detail next.

- The integration variables are linear shifts of energy, relative to the average energy of layer k.

- ERYA-Profiling uses the Landau variable **λ** as the internal integration variable, and the user can set the number of sub-divisions of one **λ to set the precision.**

The Straggling Distribution Model

- The straggling distribution are modeled after the Vavilov Distribution, from here require to be approximated by other Distributions:

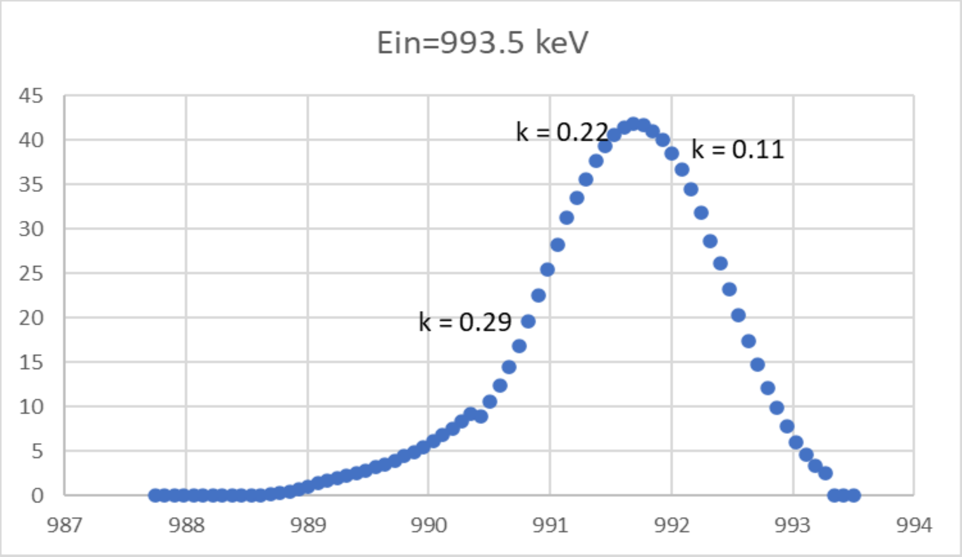
Landau k-factor	Approximate Distribution	Numerical Method
k=0	Dirac’s Function	Direct Definition
0 < k < 0.02	Landau Function	Wilkinson Formula
0.02 < k < 0.29	Vavilov-Moyal Function	Rotondi-Montagna Interpolation
0.29 < k < 22	Vavilov-Airy Function	Handbook of Mathematical Functions
k > 22	Gaussian Function	Direct Definition

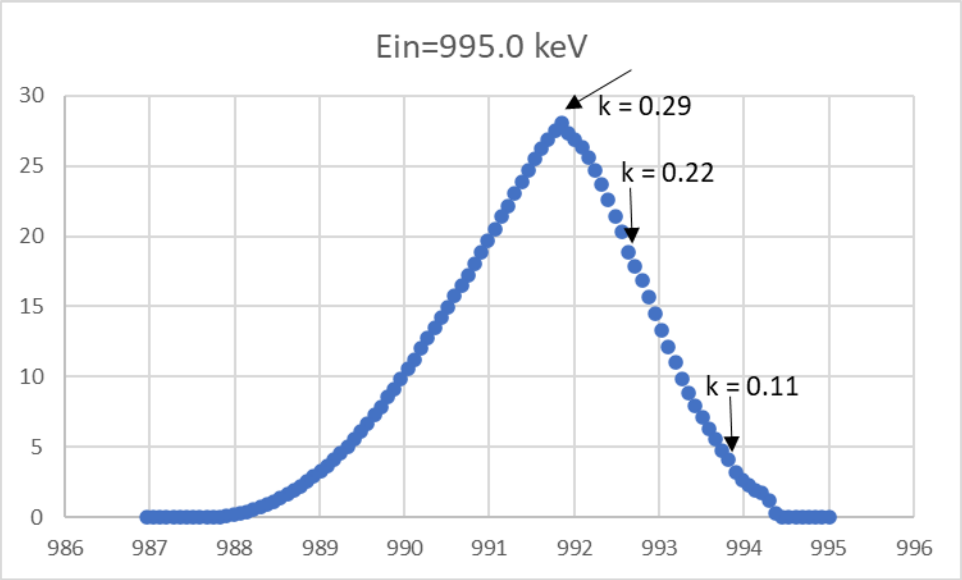
Why the Airy function as an approximation of Vavilov ?

- The parametrization of the Vavilov function are mainly based on Rotondi and Montagna paper, compared with Vavilov own published work.
- The major difference are the presence of the Airy Function of First Kind, which was the original Vavilov approximation.
- This function can be implemented as a power series where the coefficients are based on the gamma function, which can be easily implemented as a recursion formula. (Handbook of Mathematical Functions.)
- The real motive was the fact for intermediate Landau k values ($k \sim 1$), it approximates more accurately the Vavilov distribution than the Edgeworth function which is an asymptotic expansion of the Gaussian Function.

The Moyal/Airy Transition Issues

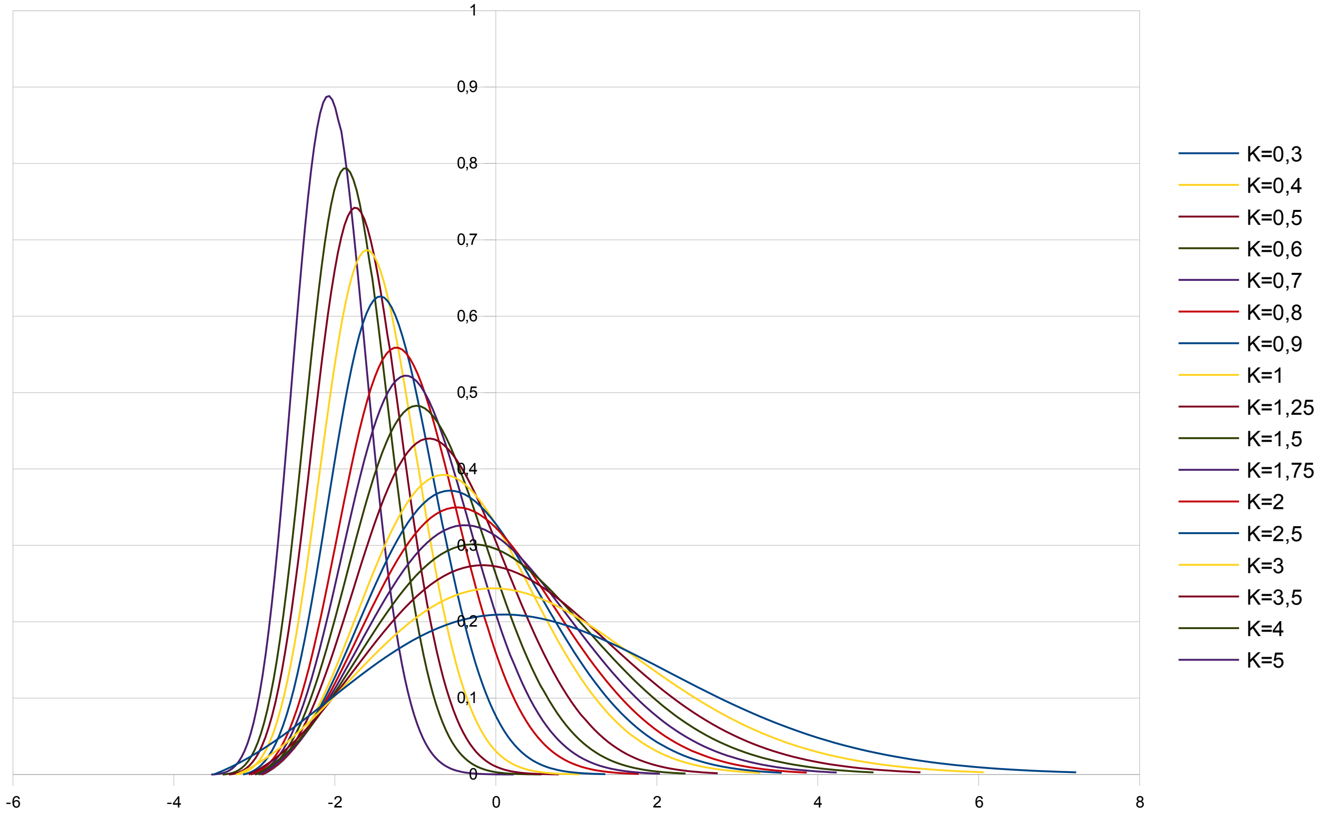
- The transition between Moyal and Airy function happens when k=0.29, but some discontinuities are inevitable, as displayed by the following yield curves:





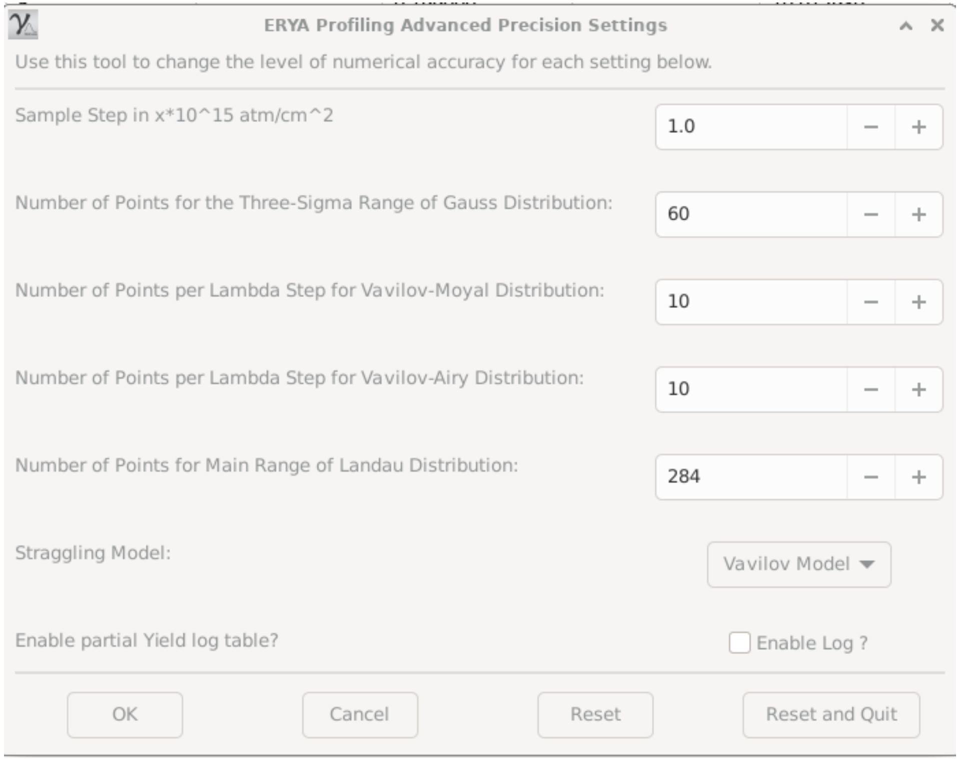
Graphical Display of the Vavilov-Airy Distributions:

- This wide set of graphical plots from the Airy Distribution reveals how the curve becomes gradually symmetric for large Landau k-factors.
- To minimize the Moyal/Airy transition issues, the Airy k-factor was a minimal cut-off of k=0.4 and replace this fixed values for k<0.4.



Full and Gauss Straggling on ERYA-Profiling

- Full Straggling on ERYA-Profiling context means that the set of approximations to handle the Vavilov Distribution are applied.
- Gaussian Straggling mode only uses Gaussian Distributions with the assumption of the asymptotic limit applied to every Landau k factor.
- The user can set this and other accuracy parameters by this widget, that are available from Advanced button:



Cross-Section handling on ERYA-Profiling I

- **Until there, it was explained about how ERYA-Profiling evaluate the yield.**
- **Since the yield are direct proportional to the cross-section, ERYA-Profiling provides four major options to encode this important physical quantity:**
  - Excitation function database (default setting), which are a compilation of IBANDL files.
  - A Breit-Wigner distribution which the user set for a limited energy interval, a Lorentzian shaped curve with fixed parameters (resonance energy and width, and the maximum value of the cross-section resonance.). Multiples peaks can be inserted directly.
  - A Breit-Wigner defined in terms of resonance strength with their energy and width.
  - A custom function defined by the user, which ERYA-Profiling provides a function interpreter.

Cross-Section handling on ERYA-Profiling II

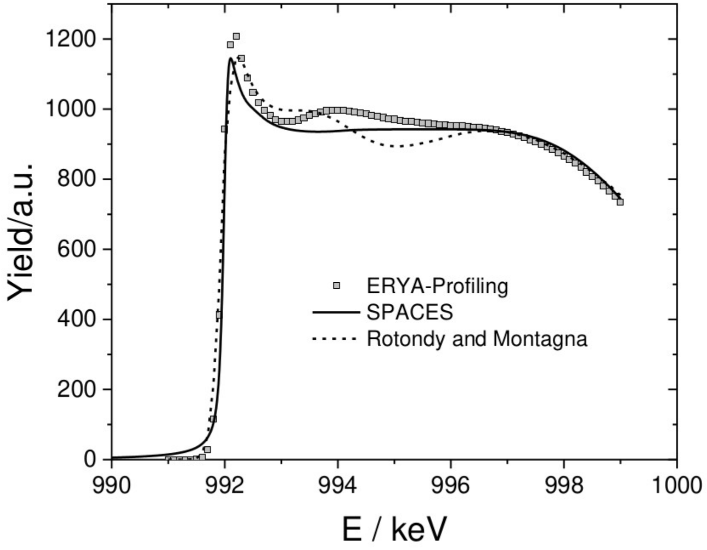
- **ERYA-Profiling evaluates the excitation function data from the database by linear interpolation between the two nearest values inside the table.**
  - The same happens for the stopping power (which are also tabular data imported from SRIM outputs), and the Detector's Efficiency if only experimental data are used.
- **Lorentzian resonances are evaluated by hard-coded formulas which depends from some parameters set by the user.**
  - The Ziegler's Parameters option for stopping power also uses a similar approach.
- **The user custom function are handled by a interpreter created by the author. This enable to convert expressions to numerical values.**
  - Detector's Efficiency and Stopping Power also supports custom functions. A debug tool similar in design to a scientific calculator widget are also available from either ERYA-Bulk or ERYA-Profiling main menu.

Other ERYA-Profiling Features

- **All default file formats to handle program settings, databases and the whole user inputs to define the sample and all physical parameters are based on XML document format.**
  - For compatibility purposes, certain files based on ASCII, including IBANDL or SRIM files, are supported within a logic of data import to XML files, or to export to ASCII files if required.
- **Excel files are directly supported by the program either to load or save.**
  - This only applies to Excel 2007 or later xlsx files (a ZIP file with XML file data), where the program author implemented this feature without any Microsoft code (but needed to follow the standard however). It only support cells with strings and numerical data.
- **ERYA-Bulk and ERYA-Profiling are open-source programs under LGPLv3 license.**

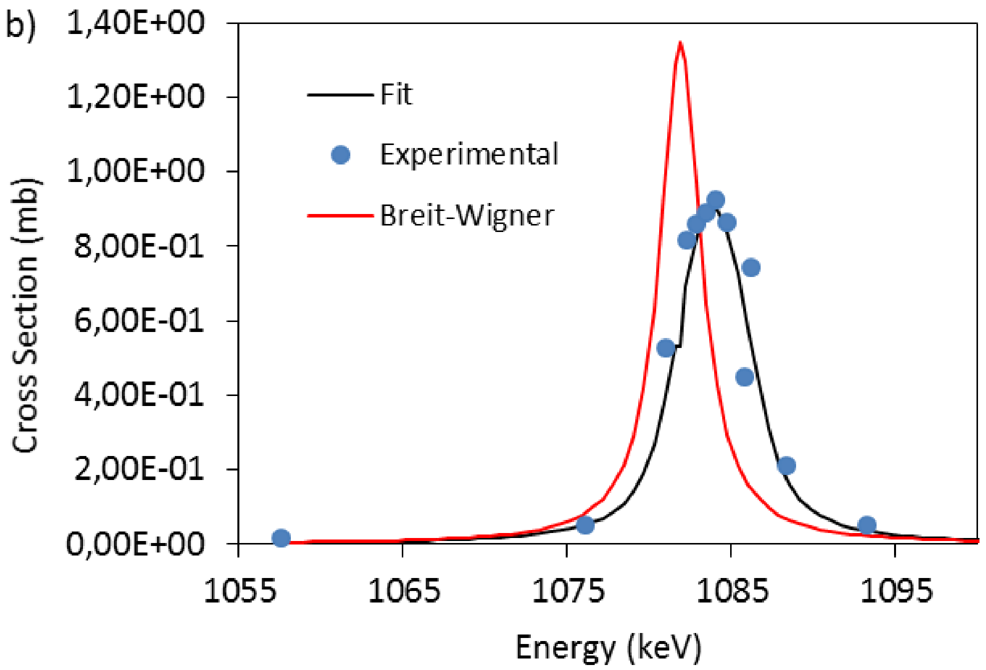
The Lewis Effect handled by ERYA-Profiling

•ERYA-Profiling under certain circumstances can predict the presence of the Lewis Peak specially for sharp resonances:



Yield from $^{27}Al(p,\gamma)^{28}Si$ reaction at 1670 keV line, where the 992 keV resonance with 70 eV width was scanned from 990 to 999 keV incident energy.
The beam dispersion is assumed to be equal to 0.1 keV.

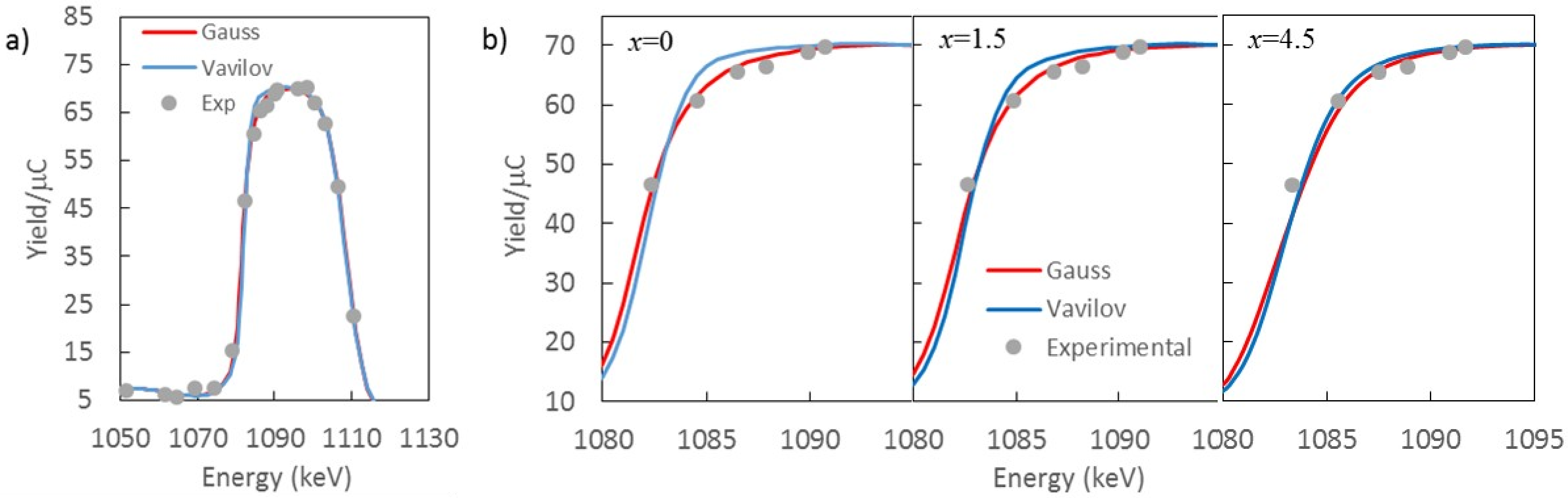
Example: Beryllium Sample with (8.50±0.15) x10^{18} at/cm^2 I



Resonance Parametrization of ^{9}Be : it display the experimental values, and their fit to a Breit-Wigner distribution.

Example: Beryllium Sample with (8.50±0.15) x10^{18} at/cm^2 II

ERYA-Profiling simulation results for a thin ^{9}Be layer with (8.50±0.15) x10^{18} at/cm^2:



It was expected a top layer of beryllium oxide, where the Gaussian straggling mode don't make any difference for the experimental data no matter the depth. Only using the Full Straggling mode, it was possible to find the depth of the oxide layer ⇒ 4.50 x10^{17} at./cm^2.

Any questions ?