

Use of the gamma function for straggling in simulation of RBS spectra

N.P. Barradas^{a,b,*}, R.P. Pezzi^c, I.J.R. Baumvol^{c,d}

^a Instituto Tecnológico e Nuclear, Estrada Nacional 10, 2686-953 Sacavém, Portugal

^b CFNUL, Av. Prof. Gama Pinto 2, 1649-003 Lisboa, Portugal

^c Instituto de Física, UFRGS, Av. Bento Gonçalves 9500, Porto Alegre, RS, Brazil

^d Centro de Ciências Exatas e Tecnologia, UCS, Caxias do Sul, RS 95070-560, Brazil

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Abstract

In standard computer codes for the analysis of RBS data, the energy straggling is taken to be a Gaussian function. This leads to unphysical simulations whenever the energy spread is comparable to the average energy loss and to the system resolution, which may happen in the near surface region. We propose to use the gamma distribution for the energy straggling, since it asymptotically approaches the Gaussian distribution for small values of the energy spread relative to average energy loss, while it has no high energy tail above the initial beam energy. This was implemented in the code NDF. We compare the results with calculations made with the stochastic model for 100 keV protons in Hf delta layers in Si and show that a major improvement is obtained with regard to the Gaussian distribution. We also show calculations for 1.5 MeV $^4\text{He}^+$ experiments.

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1. Introduction

In standard computer codes for the analysis of Rutherford backscattering (RBS) data, the energy straggling is taken to be a Gaussian function [1]. While this is often a good approximation, it leads to difficulties close to the surface, where the number of ion-electron collisions is small. In this case, if a Gaussian distribution is used for the energy loss, its high energy tail leads to a significant contribution of beam particles with energy higher than the initial beam energy. That is, some ions would have gained energy, which is clearly not the case. Instead, close to the surface the energy distribution of the ions is highly asymmetric, i.e. non-Gaussian.

One of the most reliable approaches to this problem is based on a stochastic theory of energy loss that takes into account both electronic and atomic energy transfers, which is inherently non-Gaussian [2–5]. However, even after recent progresses that led to faster calculation times, these are still too long for automated fitting or to perform data analysis with Bayesian inference using the Markov chain Monte Carlo method.

We propose to use the gamma distribution for the energy straggling, since it asymptotically approaches the Gaussian distribution for small values of the energy spread relative to average energy loss, while it has no high energy tail above the initial beam energy, similarly to the advanced stochastic approach. This was implemented in the code NDF. We compare the results with calculations made with the stochastic model for 100 keV protons in Si and show that a major improvement is obtained with regard to the Gaussian distribution. We also show calculations for 1.5 MeV $^4\text{He}^+$ RBS.

* Corresponding author. Address: Instituto Tecnológico e Nuclear, Estrada Nacional 10, 2686-953 Sacavém, Portugal. Tel.: +351 219946150; fax: +351 219941039.

E-mail address: nunoni@itn.pt (N.P. Barradas).

2. The gamma function

Firstly, we can divide the beam energy distribution $p(\sigma)$ in two components: the initial beam energy distribution $p(\sigma_0)$ and the energy distribution $p(\sigma_{\text{strag}})$ that arises as the beam crosses the sample, which we can generically call straggling, and that is our main concern here. In all cases σ is the spread of the distribution considered. In the moment where a beam enters the sample, we have $\sigma_{\text{strag}} = 0$, that is, $p(\sigma_{\text{strag}})$ is a delta function. For a sufficiently large number of ion-electron interactions the details of the energy transfer can be ignored and $p(\sigma_{\text{strag}})$ is approximately Gaussian-shaped. This is not valid for small average energy loss ΔE , where the straggling is highly skewed, being limited on the high energy side by the initial beam energy E_0 , with an extended tail (as compared to ΔE) in the low energy side. The same happens for very large energy losses if σ is comparable to ΔE , which can occur for instance at very grazing angles due to enhanced straggling at large depths due to multiple scattering [6,7].

We considered using, for the straggling, the gamma distribution with mean ΔE and standard deviation σ_{strag} , because it has the same general properties: it becomes a delta function for $\Delta E \rightarrow 0$ and it becomes a Gaussian function for $\sigma_{\text{strag}}/\Delta E \rightarrow 0$. Its general form is [8]

$$p(x) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x}, \quad (1)$$

where Γ is the gamma function, $\alpha = \bar{x}^2/\sigma^2$, $\beta = \bar{x}/\sigma^2$ and \bar{x} and σ are the mean and standard deviation, respectively. We compare the gamma and Gaussian distributions in Fig. 1 for several values of $\sigma' = \sigma/\bar{x}$, where it is clear that as σ' increases, the gamma distribution deviates more strongly from the Gaussian shape.

Note that it is only the straggling that is taken to follow the gamma distribution. The initial beam energy spread σ_0 and the system resolution are both assumed Gaussian, and

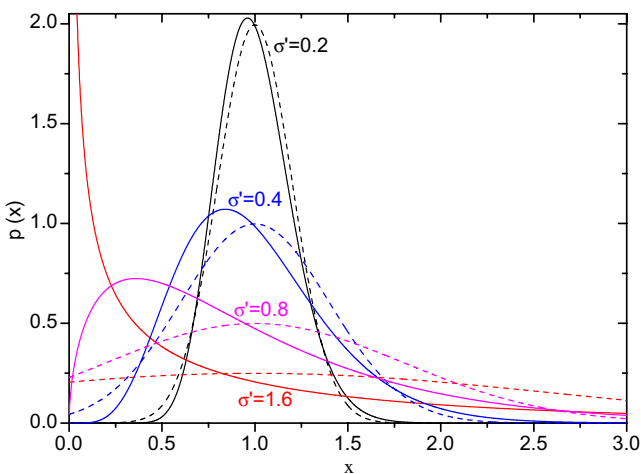


Fig. 1. Gamma (solid lines) and Gaussian (dashed lines) distributions for different values of $\sigma' = \sigma/\bar{x}$, where \bar{x} and σ are the mean and standard deviation of the distribution.

are evaluated independently from the straggling as an additional convolution.

3. Calculations

We previously developed a code, named Flatus, that implements the stochastic model of ion energy loss [9,10] and applied it to the calculation of energy spectra of Hf delta layers immersed in a pure Si matrix at different depths, ranging from 0.5 nm to 5 nm. The conditions for which the spectra were calculated were monochromatic 100 keV protons at normal incidence and 180° scattering angle, for an ideal experimental system (no beam angular divergence, point beam spot and point detector and ideal detector). The calculations are shown in Fig. 2. It is clear that very near the surface the spectra calculated with the energy distribution given by Flatus are very different from the calculation based on Gaussian energy spread. In the latter case, a high energy tail is observed, at energies larger than the maximum observable energy (97.77 keV), which is unphysical. At larger depths, which correspond to large energy loss values, $\sigma_{\text{strag}}/\bar{x}$ decreases and the calculations become more similar. It is interesting to point out that, while the total yield is the same for both distributions, the maximum yield value in the near surface part of the spectra is larger for the Flatus calculation than for the Gaussian distribution.

The important point, however, is that the calculation using the gamma distribution for the straggling is very similar to the results obtained with the full stochastic model of ion energy loss. In fact, the small differences observed between the two calculations are hardly noticeable in a real experiment. At the very least, a major improvement is obtained with regard to the Gaussian distribution.

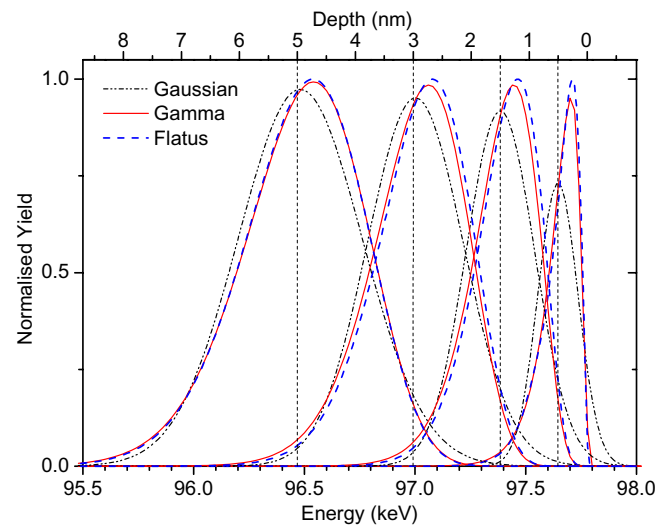


Fig. 2. Calculated energy spectra of 100 keV H^+ scattered from Hf delta layers at different Si depths, for an ideal system. Calculations using different distribution functions for the energy spread are shown: Gaussian (dash-dot-dotted), gamma (solid) and calculated by the code Flatus (dashed).

We show in Fig. 3 calculations made for 1.5 MeV $^4\text{He}^+$ at normal incidence and 180° scattering angle off Si/SiO₂ 1500×10^{15} at. cm⁻²/Au 250×10^{15} at. cm⁻², for Gaussian and gamma distributions, with straggling as given by the Bohr model [11] with the Chu correction [12,13], as calculated and enhanced by a multiplicative scaling factor. This scaling factor is an expedite way of simulating enhanced straggling. A 15 keV FWHM system resolution was used.

For a scaling factor 3, the only significant difference is in the Au signal very near the surface, where the Gaussian distribution leads to unphysical non-zero yield at energies around 1400 keV. For a scaling factor 5 to the calculated Bohr/Chu straggling, the Au signal near the surface is very different when the gamma distribution is used. In fact, the yield at the surface becomes larger than the calculation for pure Bohr/Chu Gaussian straggling, which is the well-known Lewis effect [14]. This was already observed in Fig. 2 and is a consequence of the different shape of the energy distribution. The energy distribution at different depths in the Au layer (i.e. for different values of the average energy loss ΔE) is shown in Fig. 4 for the gamma and Gaussian distributions. It is evident that the maximum yield enhancement very close to the surface (around energy 1370 keV) is due to the difference in the shape of the two

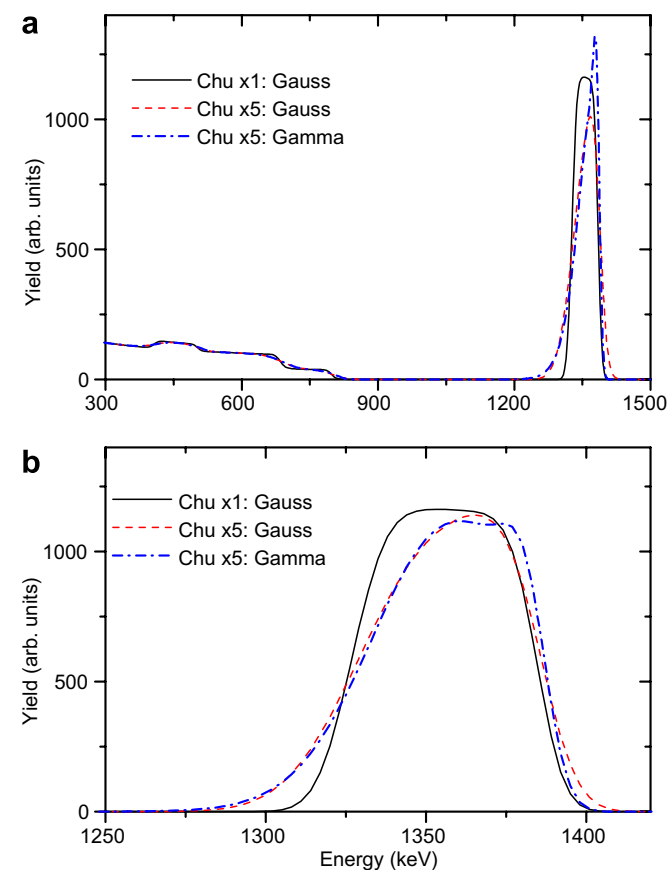


Fig. 3. Calculated energy spectra for 1.5 MeV $^4\text{He}^+$ scattered from Si/SiO₂ 1500×10^{15} at. cm⁻²/Au 250×10^{15} at. cm⁻², for different scalings of the Bohr/Chu straggling, and with Gaussian and gamma distributions.

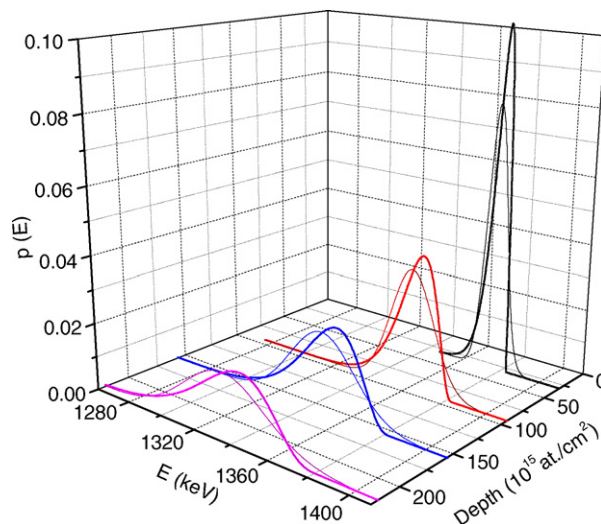


Fig. 4. Calculated Gaussian (thin solid lines) and gamma (thick solid lines) distributions at different depths, for 1.5 MeV $^4\text{He}^+$ scattered from Au.

distributions. This enhancement has been observed experimentally in medium energy ion scattering (MEIS) [9], where energy straggling is comparatively much larger than in RBS.

Finally, even for a scaling factor 5, the spectrum of Si and O are almost undistinguishable when Gaussian or gamma distributions are used.

4. Summary

We used the gamma distribution for the energy straggling in ion scattering, and showed that the results obtained in the calculation of energy spectra are very similar to those obtained when the energy distribution is calculated accurately, with the stochastic model of ion energy loss.

While we do not claim that the gamma distribution contains in itself any particular physical meaning, it leads to major improvements when compared to using the Gaussian distribution, while being almost as simple and fast to calculate.

In particular, while the Gaussian distribution leads to unphysical results near the surface whenever the energy straggling is comparable with both the energy loss and the system energy resolution, the gamma distribution does not.

We implemented the gamma distribution for the straggling in the standard data analysis code NDF [15,16], as a user option.

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