Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
Nuclear Instruments and Methods in Physics Research B 219–220 (2004) 95–98
NIM B
Beam Interactions with Materials & Atoms
www.elsevier.com/locate/nimb

Fast Monte Carlo simulation for elastic ion backscattering

P. Pusa *, T. Ahlgren, E. Rauhala

Accelerator Laboratory, Department of Physics, University of Helsinki, Gustaf Hällströmin katu 2, P.O. Box 43, FIN-00014, Finland

Abstract

A Monte Carlo method using ion packets is introduced. The method presented is optimal for the low probability scattering simulations of multiple and plural backscattering effects. Non-Rutherford cross sections are easily implemented in the framework of this model.

1. Introduction

Rutherford backscattering spectrometry (RBS) is a widely used powerful tool in determining the elemental compositions in depth of various target materials. One of the limitations of the method is multiple scattering; this effect can significantly contribute to the low energy tails of the measured spectra. This is especially the case for thick targets or low incident ion energies.

The data analysis is conventionally done simulating the spectra by using single scattering models, where single scattering yields are calculated from known scattering cross sections for ion energies at subsequent slabs in the sample. Improvements have been obtained by adding dual or plural scattering models into the simulations such as in SIMNRA [1]. Taking dual scattering effects into account, however, makes simulations very slow and problems are encountered if non-Rutherford cross sections are employed.

The scattering of single ions in various materials can be simulated using MC – techniques with programs like SRIM [2] resulting in very good agreement with experimental data. Traditional MC codes are slow in the case of ion backscattering due to the very small large-angle scattering probability. In this paper an approach using ion packets in MC backscattering simulations is introduced. The simulation time is reduced by several orders of magnitude as compared to conventional MC. A very simple fraction or packet method is presented in the case of neutron scattering in [3]. For elastic recoil detection analysis a description of an optimized conventional method can be found in [4].

2. Ion packet Monte Carlo scattering model

The idea of the ion packet MC is introduced in Fig. 1. Each scattering event divides the ion packet into two fractions: a small fraction is scattered, the remaining fraction continues unperturbed. Initial ion packet with a number of ions Q enters a sample layer. A scattering event is forced to occur within an areal density interval defined by a preset value

* Corresponding author. Tel.: +358-9-191-50064; fax: +358-9-191-50042.
E-mail address: petteri.pusa@helsinki.fi (P. Pusa).

0168-583X/$ - see front matter © 2004 Elsevier B.V. All rights reserved.
doi:10.1016/j.nimb.2004.01.034

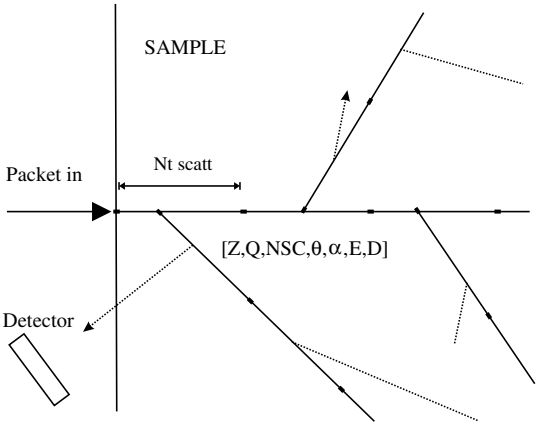

Fig. 1. Schematic illustration for a two-fold scattering simulation. Quantities in square brackets, described in text, are stored at every scattering event. Depth interval Nt_{scatt} is constant for all packet directions.

Nt_{scatt}. The scattered packet ΔQ within the path length Nt_{scatt} is the part of Q scattered outside the critical cone, determined by the critical angle θ_{c}. The critical angle is defined as the smallest scattering angle included in the calculations.

This procedure is used recursively for every packet until one of the following conditions is fulfilled: (1) the ion packet exits the sample, or (2) the energy of the ion packet has decreased below a preset minimum energy value, or (3) the number of scatterings into different directions has exceeded a preset maximum value. If the scattered ion packet is headed towards the detector, it is followed to the sample surface and recorded as an event.

At every scattering event a set of variables must be stored, see Fig. 1; depth of scattering Z from sample surface, fraction scattered Q, number of scattering events NSC, directions θ and α relative to the selected coordinates, energy of the scattered packet E and the total distance the packet has travelled D. To calculate the scattering probabilities and fractions that will be scattered, every Nt_{scatt} interval is further divided into thin slices ΔNt so that both stopping power and scattering cross section are very slowly varying (linear) functions of energy over this ΔNt. If there is a sharp resonance in the scattering cross section, the yield caused by the resonance must be averaged over the energy interval in question. Denoting an arbitrary slice by i, the part of beam packet entering this slice by q_i and the part scattered outside the critical cone and exiting from the ith slice by Δq_i:

$$\Delta q_i = 2\pi \Delta N t q_i \int_{\theta_{\mathrm{c}}}^{2\pi} \mathrm{d}\theta \sin\theta \sigma(\theta, E_i), \tag{1}$$

where $\sigma(\theta, E_i)$ is the elastic differential cross section and E_i is the energy of the ion packet in the middle of the slice. The scattering probability in the ith slice is

$$p_i = \frac{\Delta q_i}{q_i}, \tag{2}$$

and for the next slice

$$q_{i+1} = q_i - \Delta q_i. \tag{3}$$

In the interval Nt_{scatt} there are $N = \frac{Nt_{\mathrm{scatt}}}{\Delta Nt}$ slices. A function

$$\gamma_k = \sum_{i=1}^{k} p_i, \quad 1 \leqslant k \leqslant N, \tag{4}$$

is then used to locate the scattering depth in a given interval Nt_{scatt} by selecting a random number in the interval $]0 \ldots \gamma_N]$ and finding the corresponding depth. The part of beam packet scattered into a new direction from this interval is the difference of Q when entering and leaving the interval. Two more random numbers $]\theta_{\mathrm{c}} \ldots \pi]$ for scattering angle and $]0 \ldots 2\pi]$ for azimuthal angle are generated to determine the direction of scattering. The scattered packet is weighted by the differential scattering cross section of the selected scattering angle.

3. Results and discussion

The advantage achieved by packet MC compared to the conventional is based on the following. The phenomenon to be examined is the background in the backscattering spectrum, which particularly consists of ions scattered several times. Since backscattering probabilities are very small, this leads to an extremely small probability of detecting such ions. Conventional MC methods always lose the ion if it is scattered into a 'wrong' direction. The ion fraction method in such a case,

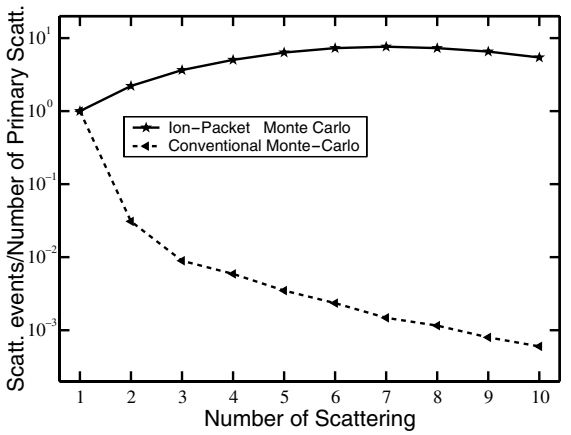

Fig. 2. Comparison between ion packet and conventional MC showing the ability to collect plural scattering events as a function of the maximum allowed scattering events. Simulations were performed with the same critical angle for both methods. Single scattering modes are scaled to unity in both cases. It must be noted that this figure is only indicative, codes like SRIM perform a huge number of small angle scatterings and are not optimized for backscattering analysis.

however, loses only a fraction of ion packet. Cumulatively the effect of this is enormous. This is illustrated in Fig. 2. In practice, any scattered ion registered as a count in the energy spectrum in conventional MC will be divided into several smaller fractions in the ion packet method. Thus, multiple and plural scattering effects with very good statistics are easily produced in the energy spectra. Table 1 illustrates scattering events detected for a single packet entering a sample when the maximum number of allowed scattering events is varied.

A spectrum simulated for 2.3 MeV protons incident on carbon is presented in Fig. 3, where elastic scattering cross section has resonant behavior. Optical model calculation was carried out with parameters taken from [6] to find the non-Rutherford elastic differential scattering cross sections at all scattering angles and energies below 2.3 MeV. The figure illustrates that the present simulation method is feasible also in the non-Rutherford case.

To demonstrate the role of the critical angle, backscattering spectra simulated for 2.0 MeV protons incident on 6 μm copper foil is presented in Fig. 4 with different critical angle values.

Table 1
Effect of the maximum number of allowed scatterings to the recorded events and calculated packets

Max. number of scatterings	Packets	Events detected
1	8	1
2	53	1
3	301	3
4	1560	14
5	6558	40
6	22,075	95
7	61,792	182
8	147,159	330
9	303,897	575
10	554,404	874

Simulation is for one packet, 2.0 MeV proton incident on 6 μm, $Nt = 51 \times 10^{18}$ atoms/cm^2 with a circular detector covering backscattering angles [162.5° ... 167.5°[. Variable Nt_{scatt} is chosen to be 8×10^{18} atoms/cm^2. Decreasing Nt_{scatt} strongly increases the number of calculated packets and events recorded at the detector.

Decreasing the critical angle value increases the computing time, but the advantage of the use of the interval scattering still remains. Discussion about the choice of the critical angle can be found in [5]. In both simulations in Figs. 3 and 4, the electronic screening was included in the calculations [7].

A disadvantage of any MC method is that non-Rutherford scattering cross sections must be known over the entire energy–angle plane in question. Also if a small Nt_{scatt} is chosen and the number of allowed scattering events is large this method requires a lot of computer memory.

4. Conclusions

Plural and multiple scattering effects often play an important role in ion backscattering experiments. In order to reliably analyze light element signals in backscattering spectra plural scattering models or MC simulations are needed. The method presented in this paper is a real time simulation with the present day computer capacity. Statistics is gained from the simulation approximately at the same rate as from a routine backscattering experiment. The method provides a useful tool for analyzing backscattering spectra or

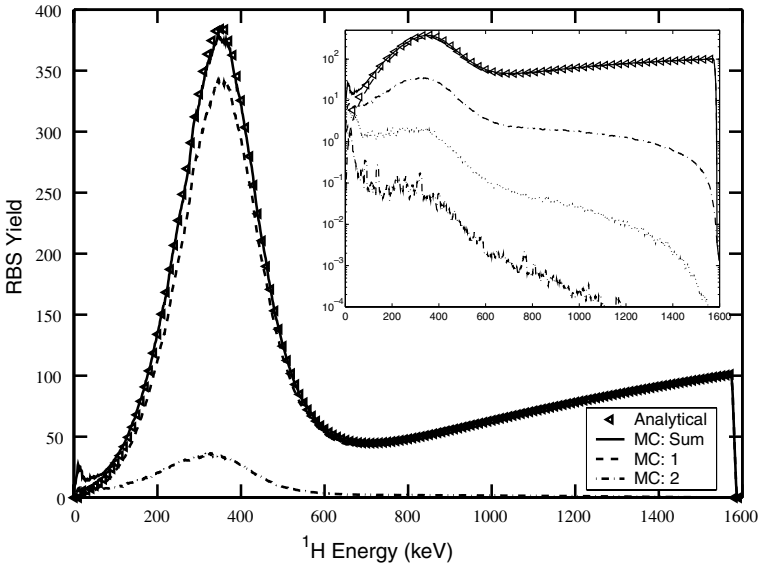

Fig. 3. Simulated non-Rutherford backscattering spectrum for 2.3 MeV protons incident on carbon and comparison with 'analytical' GISA [8] (single scattering model). Plural scattering is weak in this case and the MC and analytical spectra are almost identical. The insert also shows contribution of three- and four-fold scatterings in the logarithmic scale.

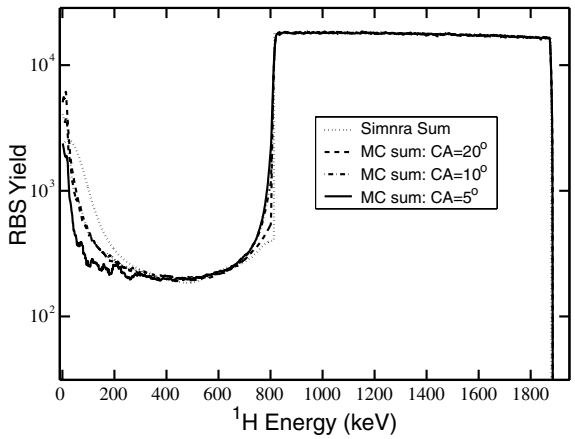

Fig. 4. 2.0 MeV protons incident on 6 μm copper calculated with different θ_c values and comparison to SIMNRA. The increase of kinematical straggling can be noted as the θ_c is diminished. The low energy tail also shifts backward. The SIMNRA simulation was calculated without straggling to indicate the differences, dual scattering contribution was added afterwards.

even for spectrum fitting. Literature data for non-Rutherford scattering cross sections are not always available and nuclear scattering models must be used as an instrument to find the scattering cross sections as a function of energy and scattering angle.

Acknowledgements

This work was supported in parts by the Academy of Finland. Support from the Finnish Academy of Science and Letters is gratefully acknowledged.

References

[1] SIMNRA computer program, http://www.rzg.mpg.de/mam/.
[2] SRIM computer program, http://www.srim.org/.
[3] I.M. Sobol, The Monte Carlo Method, Mir Publishers, Moscow, 1975.
[4] K. Arstila, T. Sajavaara, J. Keinonen, Nucl. Instr. and Meth. B 174 (2001) 163.
[5] E. Steinbauer, P. Bauer, J. Biersack, Nucl. Instr. and Meth. B 45 (1990) 171.
[6] A.F. Gurbich, Nucl. Instr. and Meth. B 136–138 (1998) 60.
[7] H.H. Andersen, F. Besenbacher, P. Loftager, W. Möller, Phys. Rev. A 21 (1980) 1891.
[8] J. Saarilahti, E. Rauhala, Nucl. Instr. and Meth. B 64 (1992) 734.