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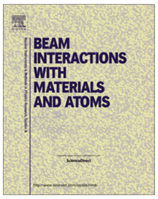

Tails

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ABSTRACT

Monte Carlo simulation software applied to ion beam analysis use the main scattering event (MSE) approximation. This approximation consist in generating ion trajectories in different directions, making the detection rate independent of the cross-section dependence on the scattering angle, therefore speeding up calculations by a factor 10^4–10^6. The event generated bear a probability weight proportional to the cross-section, so in the case of Rutherford backscattering spectrometry (RBS), events generated with a small scattering angle bear a very large weight, sometimes producing few events with a very large amplitude in the spectrum. They are avoided by setting a cut-off angle, but the signal they represent is in fact an actual contribution to the background signal. Here, it is shown that experimental spectra that include a significant contribution from several wide-angle scattering, such as tails or background signal in heavy ion RBS can be reproduced by a combination of two simulations: one featuring at least one wide-angle scattering, simulated accurately within the MSE approximation, and a background signal part, corresponding to trajectories featuring a series of small-angle scattering, simulated without the MSE approximation; this second simulation is achieved in a few minutes by increasing the detector size and mean free path by large factors, typically 100 each. The events included from the two parts of the simulation are discriminated by the minimum angle of the MSE.

1. Introduction

Ion beam analysis (IBA) simulation software has reached a high degree of sophistication in its representation of many aspects influencing IBA and difficult to account for such as setup geometry, sample structure, pile-up, non-Rutherford cross-sections (both due to interatomic potential screening or nuclear interactions), energy straggling and multiple scattering (MS) [1,2]. This was made possible thanks to theoretical developments that accompanied the development of IBA techniques in the prediction of these effects, for example regarding small-angle MS [3] or nuclear reactions [4]. One of the remaining issues is a good representation of the effect of large-angle MS, i.e. occasional deflections in an ion trajectory that are beyond the limit ("~15°") of the analytical model developed to account for MS [3]. Dual scattering calculation offered by some software already accounts for this problem up to 2nd order [5]. But in cases where the product of the cross-section times the distance travelled by the ions is large, a more detailed account of MS has to be considered. These may include heavy-ion (HI) or medium-energy elastic scattering spectrometry of a heavy target, coincidence spectrometry of thick samples, and the low energy tail in many RBS measurements.

Monte Carlo (MC) trajectory simulation, on the other hand, takes in principle full account of MS by computing all the collisions along the ions path. The problem is that the trajectory of each ion has to be simulated until a spectrum with statistics comparable to the experiment is accumulated. Without any improvement, this means simulating the trajectory of 10^9–10^{13} ions. Using TRIM [6], which already tremendously accelerates trajectory calculations thanks to the central potential, binary collision and random phase approximations, this would take up to several years-core of computing. In pioneering work, Biersack et al. developed a version of TRIM for RBS simulation [7] that was able to reproduce many features of plural scattering. To achieve this, a minimum collision angle of ~3° was set in order to limit the number of collisions to compute to a few per ion, therefore not necessarily reproducing the full effects of MS. They also considered relatively thin, heavy targets, and ions had to impinge the target normal to the surface in order to detect them along an azimuthal detector. These simulations remained long and were not covering most experimental cases of RBS neither elastic recoil detection (ERD). The main issue remains that as in experiment, only a very small fraction of the incident ions do backscatter to the detector.

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To bypass this problem, Arstila developed MCERD, a program to simulate HI-ERD spectra [8] in which he introduces two concepts: (i) to separate the computation of the ion slowdown process from that of the main scattering event (MSE), and (ii) to consider a virtual detector larger than the actual detector, then correct the trajectory of ions which hit the virtual detector so they hit the actual detector, compensating for the kinematic factor and electronic energy loss differences. The first approximation makes the detection rate independent of the angular dependence of the cross-section of the MSE, improving the efficiency of the simulation by a factor 10^4–10^6. The second concept further speeds simulations by a factor 25–100. The simulation program Corteo [9] uses these concepts (although in an independent implementation) but also manages to computes ions trajectories without calling trigonometric or transcendental functions, relying on matrices and tables stored in memory, which makes possible MC simulations of IBA spectra in a few seconds or minutes on a personal computer.

Corteo can reproduce accurately Rutherford backscattering spectrometry (RBS), ERD and coincidence spectra with arbitrarily oriented detectors [10]. But regarding Rutherford forward scattering (RFS), there is a caveat. The probability for an MSE to occur is proportional the cross-section. Hence, a particle emitted from the MSE (in the case of RBS and RFS, the same as the incident ion) transports with itself a probability weight proportional to the cross-section. If the particle leaving the MSE locus finally reaches the detector, it will increment the energy spectrum by that amount. In order to take into account all possibilities of multiple scattering, scattered ions should be produced in any direction during the MSE of each ion. However, because of the angular dependence of the cross-section, a scattered ion emitted at small angle compared to its original direction will bear an enormous cross-section, even considering a screened Rutherford cross-section (as we will see in Section 4), therefore contributing a large peak to the energy spectrum if the scattered particle finds its way to the detector through wide-angle MS. This problem is worked around by setting a cut-off angle: ions emitted below that angle will simply be rejected. (This caveat is not a problem in the case of ERD and coincidence simulations because the large cross-section events in ERD, near 90°, also correspond to small energy transfers, so these particles have very small chances to reach the detector, and if they do, would contribute to the very end of the low energy tail [8].)

For He RBS, this work-around does not significantly affect the simulation as we will see below, because of all the possible trajectories after the MSE, only those in a small cone are rejected, and they were anyway usually heading to a direction opposite to that of the detector. So they are the ones that have the smallest chances to come back to the detector. But in the case of RFS, obtained for example with an ERD setup where the forward scattered ions are also collected, the incident ions that exited the MSE in almost the same direction still have a significant chance to hit the detector, bearing with themselves an enormous probability. This contribution cannot be simply rejected because it is a non-negligible part of the FRS signal, at least in the case of heavy ions (HI) incident on layers made of heavy elements. The FRS spectrum could be useful for the sample analysis as the detection statistics are high compared to the ERD spectra, and the stopping power is high for HI, therefore providing a better depth resolution at least near the surface. But a reliable simulation has to be available in order to carry out this analysis quantitatively. HI RFS was the only case where a significant departure was found between MC and analytical simulations in the intercomparison exercise carried out a few years ago between several simulation programs [11].

Estimating correctly the amplitude of the background signal is important in order to establish properly the "charge times solid angle" product of a measurement and get quantitative depth profiles. In this paper, it is shown how a full simulation (i.e. without the MSE approximation), can reproduce the contribution of this type of events, also reproducing the low-energy tail of the spectra. However, these simulations are long. So it is shown that experimental spectra can be reproduced by the sum of two simulations: one that include the events featuring a large scattering angle (above the cut-off angle), simulated accurately within the MSE approximation (hereafter called "normal simulations"), and a background signal part, corresponding to the events with a small scattering angle, simulated without the MSE approximation (hereafter called "full simulations"); this second simulation is achieved in a few minutes-core instead of several days-core for usual full simulations by increasing the detector size and mean free path (MFP) by large factors. The two parts of the simulation are discriminated by the angle of the largest scattering event.

2. Simulation and experimental details

A complete description of Corteo can be found in Refs. [9–12]. The version 20130715 of the Corteo simulation program used here is available for download from the author's website [13] under the terms of the General Public Licence [14]. As mentioned above, Corteo computes trajectories without calling trigonometric or transcendental functions. It rather gets pre-computed values of the cos and sin components of the scattering angle during each collision along its path from tables. These tables are indexed using the binary representation of floating point numbers in a computer, as suggested by Yuan et al. [15], so the tables are logarithmically distributed in terms of energy and impact parameter, without having to compute logarithms. In version 20130715 of Corteo, the indexes include 6 mantissa bits instead of 4 in previous versions. The tables therefore use 4 times more memory. Also, for the 1% smallest values, the impact parameters are generated directly from the pseudo-random generator rather than from a list of randomly ordered values, so the widest collision angles are more uniformly distributed. These changes were necessary in order to decrease oscillations in the spectra obtained when carrying full RBS simulations, these oscillations resulting from the relatively coarse discretization of the scattering angle components evaluation and impact parameter selection.

An attempt was made to solve the problem of small-angle MSE transporting a huge probability weight by generating, for these events, a diversity of trajectory. Would an MSE occur at such an angle that the cross-section was 1000 times too large in comparison to the rest of the spectrum, 1000 ion trajectories would be generated, each bearing 1/1000th of the probability weight. Unfortunately, this method actually increases the probability to generate MSE with even smaller scattering angles, therefore amplifying the problem by several orders of magnitude. So the method was abandoned.

The simulation engine of version 20130715 produces event lists rather than a spectrum, and the user interface produces the spectrum, so the results can be analyzed in more details in separate software. If desired, the simulation engine can save many details about each detected ion, namely the locus and angles at the MSE, the impact point and angles at the detector, and a list of the few most significant scattering events along the trajectory, with the depth at which they occur. This information is useful for more detailed analysis, such as with complex detector geometry, or in order to get a better understanding of the origin and effects of MS on a particular measurement.

The simulations are compared to experiments obtained on the RBS line of the 1.7 MV Tandetron accelerator and on an ERD time-of-flight (TOF) setup installed on the 6 MV Tandem accelerator, both at the Université de Montréal. The ERD-TOF detector is placed at a scattering angle of 30° and features two timing units