Article published in Nucl. Instr. Meth. B266 (2008) 1338

Summary of "IAEA intercomparison of IBA software"

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Abstract

The International Atomic Energy Agency has sponsored a formal intercomparison exercise for the seven depth profiling ion beam analysis codes, which are: GISA, RUMP, RBX, DEPTH, DataFurnace, SIMNRA and MCERD. This intercomparison is published in Nuclear Instruments and.Methods ***B262,*** (2007) 281-303 and summarised here. The codes implement all known physical effects and they are all evaluated. We demonstrate that there is agreement between codes often better than 0.1%; and also detailed agreement with real spectra, showing in particular that the SRIM 2003 stopping powers for Si are correct to 0.6% for 1.5MeV He. For the case of heavy ion elastic recoil detection (HI-ERD) the single scattering codes performed poorly for scattered particles, although recoiled particles were calculated correctly.

PACS: 01.30.Rr; 07.05.Kf; 82.80.Yc; 34.50.Bw

Keywords: Computer software; data analysis; simulation; ion beam analysis; silicon; stopping power; channelling; channeling; RBS; EBS; ERDA; NRA; glancing geometry; Monte Carlo; straggling; roughness; multiple scattering; resonance

Background: A recent survey conducted by the International Atomic Energy Agency (IAEA)[1] showed that there are more than 200 particle accelerators in 40 countries that utilise ion beam analysis (IBA) techniques to various extents. Practitioners of IBA, and researchers who utilise IBA techniques as part of their work, are dependent on the availability and accuracy of suitable analytical software.

In 2002 the IAEA organised a technical meeting on the "Status of Software for Ion Beam Analysis in Materials Development"[2], where 12 different particle-particle analysis depth profiling software packages were identified, each using various nuclear models, nuclear data, physics and mathematical algorithms. These particle-particle software packages have been described, with a history of their development and a review of their current status[3]. This work culminated in an IAEA exercise undertaken to compare and ascertain the reliability and correctness of the outputs of seven different particle-particle analytical software codes, and the present paper is an of this work. The IAEA organised a final meeting between the participants in October 2005. During this meeting, and the subsequent follow up, participants corrected or improved their calculations. The purpose of this work is to report on the current state of the codes, including all their best capabilities, and we present here an extended abstract of the final results obtained[4]. The usability (ease of use) and documentation of the codes were not assessed. PIXE and PIGE (particle induced X-ray and gamma emission) were also not discussed in this paper, the IAEA having previously reviewed the status of gamma ray analysis software packages[5] and PIXE analysis software packages [6]. PIXE of course is not primarily a depth profiling technique; nor is PIGE in the many cases where the cross-sections do not have resonances.

Participating codes are GISA [7], RUMP [8], RBX [9], DEPTH [10], DataFurnace (NDF) [11], SIMNRA [12], and MCERD [13]. The main purpose of all these codes is to enable elemental depth profiles to be inferred from particle scattering spectra. The first three codes are "first

generation codes", initially designed to do efficient and accurate simulations of single RBS spectra where multiple scattering is not significant. DEPTH is designed as a code for making the best possible calculation of energy straggling effects. It is not really designed as a spectrum calculator, although it was used as such for this work. NDF and SIMNRA are new generation codes which are designed to handle all cases of interest at the best possible accuracy. NDF depends on DEPTH for energy straggling calculations. It is worth remarking that, although they were developed completely independently, in most cases the results for NDF and SIMNRA are almost identical (and the larger differences are usually explicable in terms of the algorithm treatments).

MCERD is designed specifically for ERD where the assumption of single scattering is usually a poor approximation: it is a Monte Carlo code using a binary collision approximation that naturally takes multiple collisions between incident ions and target atoms into account, while all the other codes utilise versions of the standard simulation procedure first described by Ziegler et al. [14], where ion trajectories are approximated by straight lines, and only a single scattering event is considered. Multiple collisions can be approximated by some of the single scattering codes (RBX, DEPTH, NDF, SIMNRA) as an additional energy broadening contribution, and some of these codes also calculate the yield due to double scattering (NDF & SIMNRA). MCERD uses a very efficient algorithm to give reasonable calculation times, even though it is an MC code. In ERD, glancing incidence together with glancing exit geometries are typical, and it is in these cases, especially when heavy ions are used, that multiple and plural scattering must be correctly taken into account to be able to quantitatively reproduce the spectra.

Quantitative intercomparison between codes: The most important factor affecting spectral shape is the absolute value of the scattering and stopping cross-sections used. For traceable work it is essential that the code user can supply these cross-sections (where they are non-Rutherford) directly to the code. For accurate work it is important that a modern compilation

of stopping powers is accessible to the code, and we agreed to use the SRIM 2003[15] stopping power database. All the codes could accept arbitrary scattering cross-sections, but the oldest code, GISA, although giving reasonable results, could not implement SRIM 2003 in time for the exercise and therefore used SRIM 1991 [16].

We started by checking that all the codes agreed when calculating the 1.5MeV $^4He^+$ RBS (Rutherford backscattering) spectrum from a {Si bulk / SiO_2 200nm / Au 50nm} target with a reasonable detector energy resolution and Bohr straggling, but no screening or pileup. The single scattering codes agreed excellently with MCERD (which was not designed primarily for RBS), validating the MonteCarlo approach. The single scattering codes agreed to better than 0.3% on the yield and height of the various features of the spectrum, and the RUMP/NDF/SIMNRA subset agreed within 0.1%. For the various edge (surface and interface) signal positions this subset agreed at about 100eV, and for the various edge widths NDF and SIMNRA agreed at 500eV.

The same comparisons were made for the same target, but using 3.5MeV $^7Li^+$ HI-RBS (heavy ion RBS). Again, MCERD agreed excellently with the single scattering codes, but for these agreement was not so good as for He-RBS: it was between 0.2% and 0.7% for the yield and height of the various features of the spectrum, and the RUMP/NDF/SIMNRA subset agreed within 0.3%. For the various edge (surface and interface) signal positions this subset agreed at about 700eV (and RUMP/SIMNRA agreed at 200eV), and for the various edge widths NDF and SIMNRA agreed at 800eV.

A similar comparison was made for a {Si bulk / CD_2 150nm / CH_2 150nm / CD_2 150nm} target using 1.8MeV $^4He^+$ ERD and a 6μm mylar range foil to stop the scattered incident beam. The agreement between the codes was much poorer, but for the RUMP/NDF/SIMNRA subset it was better than 0.4% for the yield of the D and H signals. NDF and SIMNRA agreed at 0.1% for the signal yields, at 400eV for the signal positions and usually better than about 800eV for the signal widths.

Qualitative intercomparison between codes: Heavy ion ERD with glancing incidence geometry was simulated for a 50 MeV $^{127}I^{10+}$ beam on the Si/oxide/Au sample, first without multiple scattering for which all the codes agreed quite well; with NDF, SIMNRA and MCERD being almost indistinguishable. The same simulation for a realistic ToF (time of flight) detector could be done only by SIMNRA and MCERD, which agreed excellently. However, the inclusion of multiple scattering is a very hard case: it plays an important role, including changes in total yield[17] which has a large error on the scattered I signal for all the single scattering codes. NDF and SIMNRA gave very similar results, but were not better than RBX and DEPTH at matching MCERD (which is known to simulate this case well). RBX and DEPTH produce a spectral shape closer to that of MCERD than do NDF or SIMNRA because they treat the shape of the energy distribution as a Pearson VII function which NDF and SIMNRA approximate as a Gaussian.

NRA (nuclear reaction analysis) calculations were made for near normal incidence and exit beams with NDF and SIMNRA, both for the $Si/CD_2/CH_2/CD_2$ target with the same stopper foil and the $d(^3He, ^4He)p$ and $d(^3He,p)^4He$ reactions, and for a bulk FeN_4 target with the $^{14}N(d, ^4He)^{12}C$ reaction. The latter case involves inverse kinematics which must be handled correctly. For both cases the agreement was excellent.

The inclusion of electronic screening in the scattering cross-section did not significantly change the (small) differences between the codes, and nor did the calculation of different geometries or a smoothly varying concentration profile. We also checked the effect of ultra-high resolution detectors (where the resolution is comparable to the channel width, which has some computational intricacies), and the codes are close, with RUMP, NDF and SIMNRA very close.

Pulse pileup could be calculated only by RUMP, NDF and SIMNRA. NDF and SIMNRA implement the accurate algorithm of Wielopolski and Gardner[18] and give

comparable results. RUMP uses a different algorithm but gave very similar results as shown for a real a-Si spectrum..

Energy straggling, including contributions from multiple scattering and geometric broadening as well as Bohr straggling with the Chu correction[20] , could be calculated only by DEPTH, NDF (using the DEPTH calculation), SIMNRA and MCERD. These all give very similar results, as expected since they handle the effect of multiple scattering similarly[21]. The main contribution to plural scattering is double scattering, which only NDF [22] and SIMNRA [23] can calculate (and only for RBS). These agree surprisingly well, and also give results remarkably close to MCERD for a non-glancing geometry and 1.5MeV He. However, unsurprisingly, for a glancing incidence and exit geometry with this beam the single scattering codes do not calculate double scattering very well.

Elastic (non-Rutherford) backscattering (EBS) is a special case, since it frequently involves very sharp resonances in the cross-section function which must be handled very carefully. For the case of a broad resonance (the Si substrate signal of the Si/oxide/Au target with a 1.8MeV H beam) NDF and SIMNRA are almost indistinguishable, GISA is close and RUMP, RBX and DEPTH are fairly close. The case of a sharp resonance is considered by using a He beam on the same target with an energy close to the O resonance at 3.05MeV. Even though this resonance is not buried deeply in the sample the agreement between RUMP, NDF and SIMNRA is only 4% at the peak of the O signal. RBX and DEPTH do not reproduce the shape of the resonance very well. For this case the algorithm used by NDF is demonstrably superior, as shown by the good fit to the deeply buried ultra-sharp resonance at 1483keV for protons on Mg^{24}.

The important case of channelling could be treated only by RBX. We considered a 100% substitutional 66keV 10^{16} Ge/cm^2 implant into bulk (100)Si, assuming a point defect distribution in the Si following the Ge distribution but with a 2% maximum concentration, and also assuming a perfect (unreconstructed) surface with the Si bulk lattice constants. RBX gave

results quite closely similar to a good Monte Carlo calculation by the code BISIC [25] which is designed specifically for channelling in Si, SiC, and SiGe.

Quantitative comparison with real spectra: Real spectra were also analysed by the codes, except DEPTH which is not designed for spectral analysis. First, as a sanity check, a spectrum from an amorphous Si sample was simulated. This spectrum has been specified with great detail and accuracy[26], and we found excellent agreement between it and the simulations for all the codes (including DEPTH: this is the only real spectrum simulated by DEPTH; DEPTH was not used to simulate the other real spectra discussed below).

The fluence (relative to SRIM2003 stopping) of an 80 keV Sb implant into a (100) Si wafer with a 90 nm surface oxide amorphised to 630nm was determined for all the codes from two spectra collected simultaneously. The two spectra had charge.solid-angle products of 0.845μC.sr and 2.31μC.sr and are shown in Fig.1. The material has a certified retained Sb content (1σ uncertainties) of $48.1(3).10^{15}$/cm^2 [27]. Our average result was $48.015(55).10^{15}$ Sb/cm^2, which is extraordinarily (and accidentally) close to the certified value. This means of course that the SRIM 2003 stopping powers happen to be correct for this beam and target. What is astonishing is that the standard deviation of our Sb fluence determination is just over 0.1%, which is comparable to the counting statistics uncertainty of the Sb signal (0.05%).

A spectrum from a nominally HfO_2 layer on Si was analysed by all the codes. Close results were obtained from all the codes but we consider here only those codes that used SigmaCalc cross-sections for O [28]. The composition determined is $296(4).10^{15}$ Hf/cm^2, a 1.4% variation, and $599(5) \times 10^{15}$ O/cm^2, a 0.8% variation. The variation expected from counting statistics is 0.2% for the Hf signal and 4.5% for the O signal. All the analysts correlated the Hf and O signals thus trading a larger than expected uncertainty for the Hf signal for a smaller than expected uncertainty for the O signal. There is also a Zr impurity at 1% relative to Hf, which was determined at 2.7%, comparable to the 5.6% expected from counting statistics.

Multilayers with nominal structure Si bulk / Re 5nm/(Co 2nm/Re 0.5 nm)$_{15}$ were produced by magnetron sputtering, and analysed both manually [29], and with NDF [30]. The objective of this analysis is to test the ability of retrieving both the very complex layer structure and the roughness. A set of six spectra were collected, from near-normal incidence to grazing incidence, with beam incidence angles with respect to the sample surface down to 6º. Only NDF and SIMNRA reported on this case. NDF found average layer thicknesses of 356(30).10^{13}Re/cm^2 and 207(17).10^{14}Co/cm^2, and SIMNRA found 368(31).10^{13}Re/cm^2 and 227(13).10^{14}Co/cm^2. The average difference between NDF and SIMNRA (discounting the systematic difference) is 28pm for the Re layers and 94pm for the Co layers. Both codes find that the substrate has a quantifiable roughness with a conformal layer structure. The roughness is consistent with a substrate feature height and width of about 0.6 nm and 40 nm. This is excellent agreement with astonishingly precise information available from a standard RBS sytem considering that the depth resolution is usually considered to be of the order of 10nm.

Acknowledgements

We would like to thank the IAEA for supporting this intercomparison exercise, Dr. Alexander Gurbich for providing some scattering cross sections, and Dr. Mitsuo Tosaki for providing the carbon data. Work is partially supported by the Hungarian OTKA grant No.: T 046238 and the UK EPSRC grant GR/R50097.

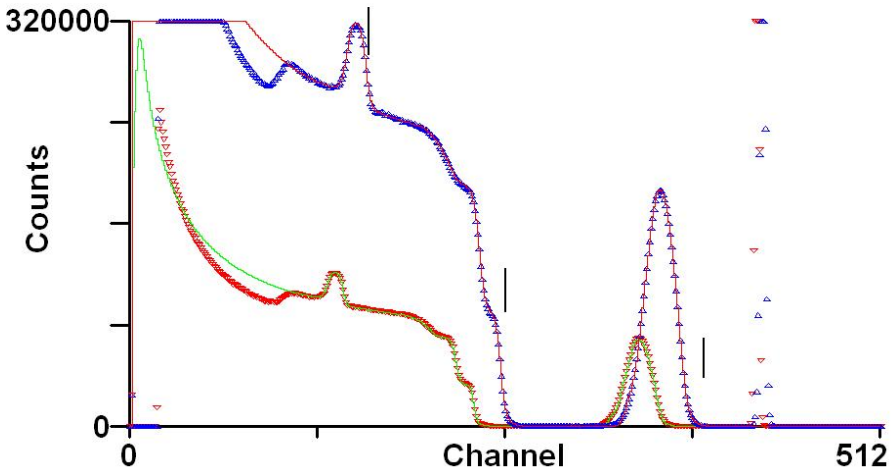

Fig.1: Two fitted spectra collected simultaneously from the IRMM Sb implanted and amorphised certified standard with 1577keV $^{4}He^{+}$ beam and two detectors at 170° and 150°. Symbols=data; lines=fits. The fits from all the codes are indistinguishable. The Sb, Si and O edge positions are marked for the larger detector. The beam is channelled on the substrate (reducing yield at low energies and ignored in the fits) and the electronic pulser is visible for both spectra near channel 430.

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