IAEA Consultant's Meeting on Inter-comparison of PIGE codes (II): depth-profiling

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IAEA, Vienna

Minutes

Participants: N. P. Barradas (IAEA/Physics), J. Cruz (Univ. Nova Lisbon), P. Dimitriou (IAEA/Nuclear Data), V.M. Manteigas (Univ. Nova Lisbon), M. Mayer (MPI-Garching).

1. Motivation

The purpose of the meeting was to perform a detailed inter-comparison of the performance of the four available PIGE analysis codes, ERYA-profiling, NDF, SIMNRA, and SPACES, in simulations of multi-layered samples, i.e. depth profiling.

Seven exercises were defined by J. Cruz (Lisbon) with input from other participants to investigate how the codes perform in simulations of:

- a thin film plus substrate (substrate can be heavy or light element)
- two films plus substrate (substrate can be heavy or light element)

under the following conditions:

- constant cross sections or a single sharp resonance or several sharp resonances
- (a) full beam straggling and (b) Gaussian-type spread
- different film thickness (surface, deep, very deep)
- stopping powers from SRIM2013

The exercises are provided in Annex 1.

Participating codes:

ERYA-Profiling: J. Cruz
NDF: N. Barradas
SIMNRA: M. Mayer
SPACES: I. Vickridge - only in Exercise 2 with full beam straggling since the code is suitable for sharp resonances and thin layers.

2. Presentations

Participants presented the main methodology and physics implemented in the codes for simulations of multi-layered samples, as well as the important approximations. Presentations are available on the meeting website: https://conferences.iaea.org/event/382/

3. Results

After the code presentations, P. Dimitriou presented a detailed graphical inter-comparison of the results of the codes for the seven exercises. The main remarks for each exercise are listed below:

Exercise 1: thin Al film [] on a thick Si substrate using a fictitious constant cross section. The aim of the exercise was to test the algorithms implemented in the codes for different beam straggling models and beam energy spreads.

The relative differences between the three codes were very small with ERYA giving the most stable results. The differences between ERYA and NDF are of the order of a few ppm while SIMNRA varies by up to 50 ppm. Similar results are obtained for all four sub-cases, i.e., with full and Gaussian beam straggling, and with DE=0 and DE=1 keV spread.

Exercise 2: thin Al film [] on a thick Si substrate using a fictitious Breit-Wigner thin resonance. The aim of the exercise was to test how the codes perform with a single thin resonance for different beam straggling models and energy spreads.

The initial results showed that for full beam straggling with DE=0 keV, NDF produces a rather pronounced Lewis peak compared to ERYA while SIMNRA does not show a peak. In addition, ERYA underestimates the plateau after the Lewis peak.

The ERYA calculations with beam energy spread DE=1 keV were performed with DE=1 keV as the standard deviation while the other codes used 1 keV for the FWHM. As a result, the ERYA slopes were not as steep as those given by the other codes.

ERYA code also calculated the B-W resonance using the given resonance parameters rather than reading the tabulated cross section like the other codes, which led to some differences.

In these calculations, SIMNRA may be sensitive to the detailed shape of the distribution functions, while NDF may be sensitive to the sub-division of sub-layers.

Relative differences between the codes ranged between a few percent to a few 10 percent with the largest differences being around the Lewis peak.

In addition to the calculations with an energy step of 500 eV, the exercise was also performed with 50 eV energy step. The results were compared with the results from SPACES for full beam straggling.

The comparison confirmed that NDF produces a too pronounced Lewis peak that is shifted to lower energies especially in the case of DE=1 keV energy spread compared to SPACES. SIMNRA does not produce a Lewis peak while ERYA clearly shows a peak, however, the results show oscillations that need to be further investigated.

Exercise 3: thicker Al film (3.27 μm) on a thick Si substrate using a measured cross section featuring several sharp resonances. The aim is to test the codes performances with several sharp resonances with different beam straggling models and beam energy spreads.

All the codes agree in shape and magnitude with relative differences of the order of a few percent in the case of full beam straggling without energy spread that drop to a few parts per thousand or even less in the case of Gaussian straggling. Although the differences are very small, in the case of full beam straggling they need to be investigated as they we would expect the codes to agree as in the case of Gaussian straggling.

Exercise 4: The same as Exercise 3 but for a thin Al film (0.98 μm) on a thick Si substrate and in a different energy range that is close to the sharp resonance.

Larger differences are found between SIMNRA and the other codes for full beam straggling while for Gaussian straggling larger differences are found between ERYA and the other two codes. Overall, the largest relative differences arise for full beam straggling calculations while for Gauss straggling the differences are of the order of 1% maximum.

Exercise 5: The results are qualitatively similar to Exercise one and are affected by the same features in the calculations.

Exercise 6: Thin Al film sandwiched between a thicker Si substrate and bulk Si and a sharp Breit-Wigner cross section. The aim of this exercise was to test the performance of the codes for straggling effects caused by crossing the surface Si layer.

Some of the differences between the codes have already been mentioned above. What is noticeable here is the difference between NDF which gives larger yields compared to the two other codes and shows a dip at one energy point (2002 keV) when using Gauss straggling with 0 keV. These features could be due to numerical instabilities and will be further investigated.

Exercise 7: Thin Al film sandwiched between a thicker Si layer and bulk Si substrate with a measured cross section featuring several sharp resonances.

The differences observed between the codes are below 6% and need to be investigated.

Following the above comparisons and observations, the following changes were made in the calculations and/or the codes:

ERYA:

- ΔE=1 keV spread was initially treated as a standard deviation and not as FWHM of the Gauss distribution. It is now treated as a FWHM of the Gauss spread function.
- The sharp fictitious resonance was originally calculated analytically using the given parameters. It is now read from the given table.
- Both the internal layer thickness and Landau parameter is being optimized.
  The first two changes brought the ERYA calculations in line with the other two codes and led to significant improvement in most cases.

NDF:

- Included Tschälär effect in all Gaussian calculations.
- No longer interpolate the cross section to zero keV, now zero cross section outside the range given in the R33 file is assumed.
- Did not use automatic subdivision of layers in Exercise 6 at 0 keV – which led to the dip at 2002 keV.

SIMNRA:

- Improved accuracy of integration of cross-section times straggling from about 1E-5 to about 1E-6 which improved the results of Exercises 1 and 5.

The above-listed changes improved the calculations in some of the cases, reducing the differences to numerical fluctuations that have no physical bearing, especially in the cases where Gaussian straggling model was used. The final revised results of this round 1 comparison are available on the meeting website.

However, in the case of the full straggling model, the implementation in NDF needs to be revisited as the PIGE routine used in round 1 is not correctly implementing the Chu straggling values. In addition, the performance of SIMNRA around the Lewis peak in exercises 2 using the 50 eV energy step needs to be further investigated, as does the oscillatory behaviour of ERYA in the plateau after the Lewis peak.

This led to the decision to perform a second round of calculations.

Round 2 of calculations:

Calculations of exercises 1 to 7 will be repeated after the following changes have been implemented in the codes:

ERYA:

- stopping power tables: increase number of points in the tables.
- full straggling curves: introduce a smoothing procedure at the k values where the straggling functions change.
- Gaussian integration limits: 3 standard deviations to 5 standard deviations.

NDF:

- Correct the Chu implementation.

SIMNRA:

- Improve accuracy of asymmetric energy loss function close to the surface, where the straggling distribution is strongly asymmetric.

4. Next steps

The second round of calculations will be submitted by 31 March 2024.

Following that, an online meeting will be held to discuss the results and finalize the conclusions and recommendations. The layout and details of the publication will also be agreed.

Possible dates: week 22-26 April 2024.

All code developers will be invited to participate.