Computer Simulation of Ion Beam Analysis Methods

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Ion beam analysis (IBA) methods are powerful tools for depth profiling of elements and isotopes in the near-surface layer of solids. These methods are quantitative, do not suffer from matrix effects, and are non-destructive. However, the quantitative evaluation of energy spectra obtained by IBA methods usually requires the use of sophisticated computer codes. Four different types of codes were developed during the last three decades for this purpose [1, 2]: Analytical codes (SIMNRA, NDF, and other), Monte-Carlo (MC) codes with weight function (MCERD, CORTEO), full Monte-Carlo codes (SDTrimSP, SRIM), and molecular dynamics (MD) codes (MDRange and other).

Analytical codes are well developed, fast, versatile and can simulate quantitatively most IBA methods. A number of codes has been intercompared and yielded very good agreement, thus giving some confidence in their correctness. Nevertheless, some phenomena, such as multiple small-angle scattering, plural large-angle scattering, or surface roughness can be taken into account only approximately by this type of codes.

MC codes provide improved accuracy, but at the cost of increased computing time. MC codes with weight function were developed for IBA with MeV ions and are fast enough for spectrum simulation. Full MC codes are a more accurate alternative, but are suffering from long computing times, rendering their use impractical even with modern computer hardware. MD codes have been used successfully for the simulation of channeling in single-crystalline targets, but computing times are still too high for full spectrum simulation.

Current developments are especially focusing on the following areas:

- Improved simulation of channeling spectra,
- combined evaluations of measurements with multiple detectors and/or different methods,
- analysis and simulation of 3-dimensional structures,
- application of artificial intelligence and machine learning for the interpretation and evaluation of IBA spectra.

References

[1] E. Rauhala et al., Nucl. Instr. and Meth. B 244 (2006) 436

[2] M. Mayer et al., Nucl. Instr. and Meth. B 269 (2011) 3006