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RUTHELDE - A Differential Evolution Based RBS Spectra Fitting Algorithm and its Capabilities Beyond Fitting

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Recently, we applied evolutionary optimization, namely differential evolution, to fit Rutherford backscattering spectra [1]. We derived an algorithm that is capable of finding, with very high precision, the sample composition profile that best fits the experimental spectra in an autonomous manner. The robust nature of the differential evolution algorithm, especially with respect to the rather low increase of computation time with increasing number of free parameters, not only results in an excellent performance in standard fitting operation but also enables the introduction of additional fit parameters. Thanks to the stochastic nature of the optimization algorithm the code benefits well from the multi-thread/multi-core implementation.

The stochastic nature of the optimization algorithm naturally also lends itself to determining the uncertainties of the results, namely the layer areal densities, the elemental ratios and the detector calibration. Besides, it becomes feasible to predict the expected accuracy of an RBS experiment for given experimental conditions (e.g. scattering geometry, accumulated charge, etc.) prior to the actual measurement. Vice versa, the code allows us to determine what experimental conditions would be required to achieve a certain accuracy in the measurements.

Further, by adding the correction factor to the stopping cross section(s) of the projectile ions as a free fit parameter we demonstrated RUTHELDEs capabilities to derive the stopping cross sections with high precision from RBS measurements [2]. This approach opens new opportunities to determine stopping cross sections.

In our recent work, we have introduced the ability to apply non-Rutherford cross sections in RUTHELDE. This feature will broaden the applicability of the software. Besides, by making the primary ion energy a free fit parameter, it is expected that RUTHELDE will open a new opportunity to realize the energy calibration of ion accelerators by utilizing well known resonant reactions.

In this presentation we will summarize the mechanisms of the code, show certain examples of target model determination, uncertainty calculations and contributions to stopping cross section measurements [2]. We will present the corresponding open-source software package and demonstrate its capabilities, features and limitations.

References

[1] R. Heller et al., J. Appl. Phys. 132 (2022) 165302; https://github.com/DrReneHeller/Ruthelde
[2] J. Meersschaut et al., Nucl. Instrum. and Methods in Phys. Res. B 553 (2024) 165406

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