THRESPECT – A COMPUTER PROGRAM FOR THE THRESHOLD ENERGIES DETERMINATION

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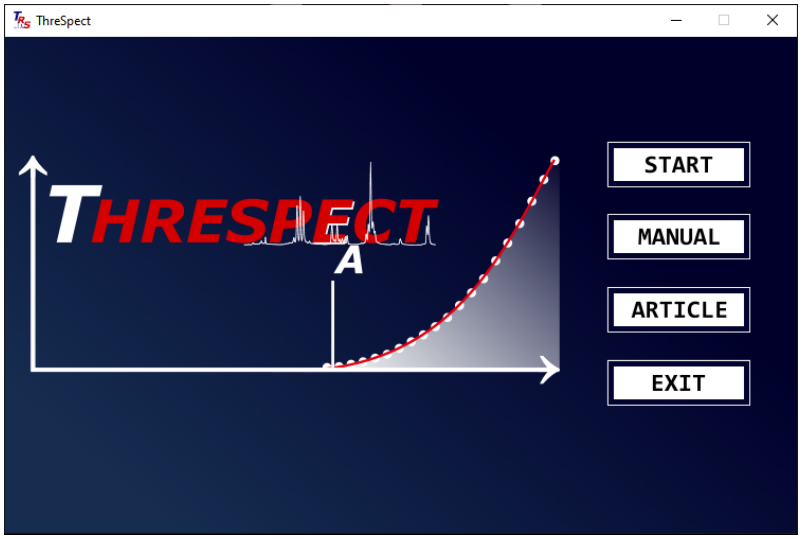


In the present communication, we present a proprietary computer program, "ThreSpect," dedicated to determining the threshold energies, E_A. A theoretical E_A closest to the actual value can only be obtained by programming the mathematical functions and performing a fully automatic fitting process utilizing iterative non-linear optimization algorithms. Our approach involves programming the convolution of Gaussian and Wannier functions and employing the Trust-Region-Reflective Least Squares algorithm to solve the curve-fitting problem. The program's interface, functionality, and examples of determining the threshold energy of some compounds known from the scientific literature are briefly presented.

THEORETICAL BACKGROUND

The convolution of the Gaussian function with the standard Wannier function produces a modified Wannier function ($w*g$) that expresses how the shape of $w(E)$ is modified by the $g(E)$ radiation beam energy distribution:

$$(w * g)(E) = (aE_x + b) + \int_{E_A}^{\infty} \left[\frac{1}{\sigma_G \sqrt{2\pi}} e^{-\frac{(E_x-\mu)^2}{2\sigma_G^2}} \right] [\sigma_W (E_x - E_A)^n] \, dE_x \, . \quad (1)$$

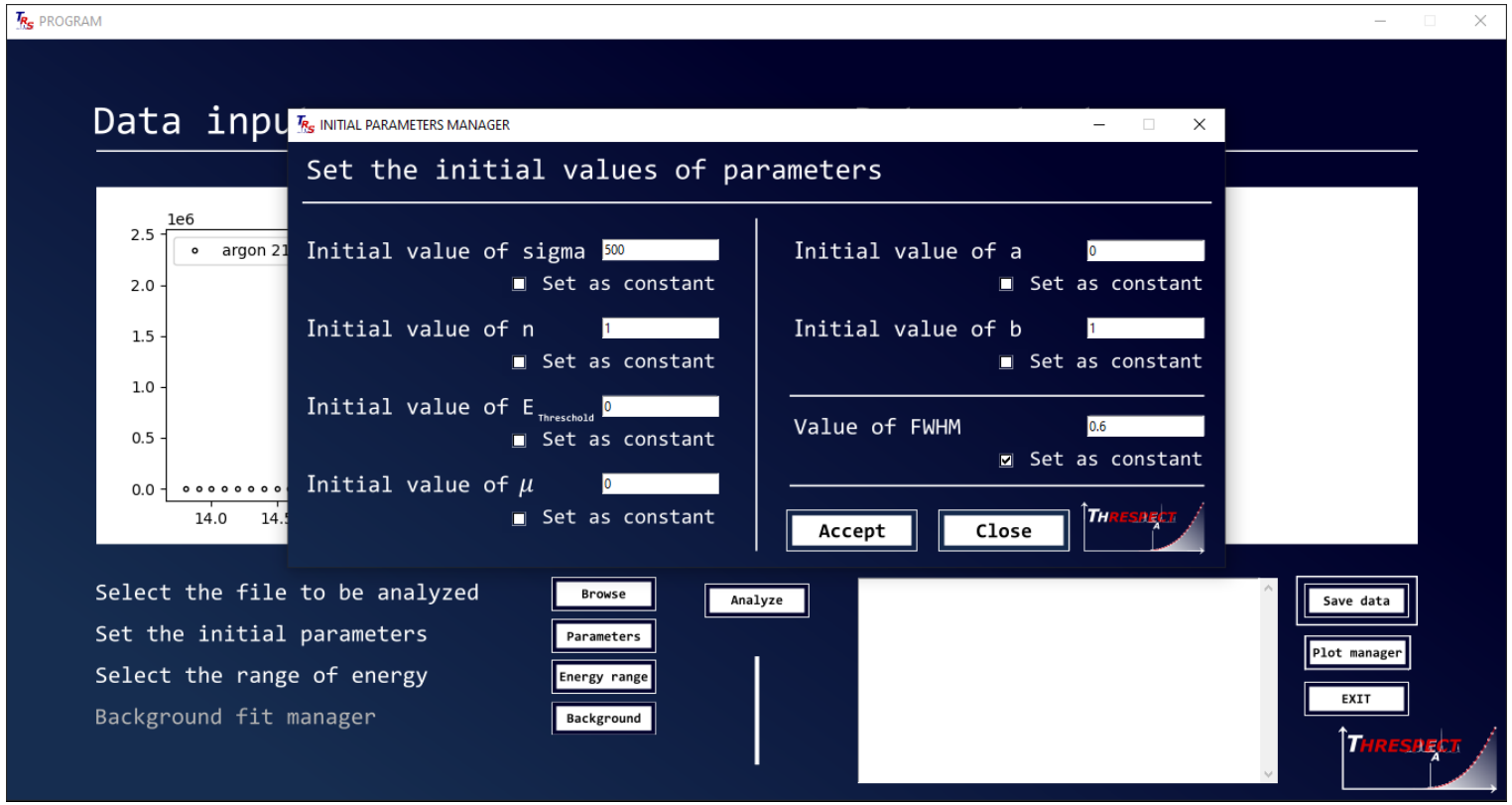
Here, the σ_G parameter is related to the full width at half maximum (FWHM) of the peak according to the relation:

$$FWHM = 2\sqrt{2 \ln 2} \, \sigma_G = 2.3548 \cdot \sigma_G \, . \quad (2)$$

Expression (1) allows determining threshold energies E_A and n-Wannier exponents of various products from the fittings to the measured cross-section curves irrespectively whether the species are generated from collisions with electrons, ions, or photons and detected with mass spectrometric or emission spectroscopic techniques.

PROGRAM FUNCTIONALITY

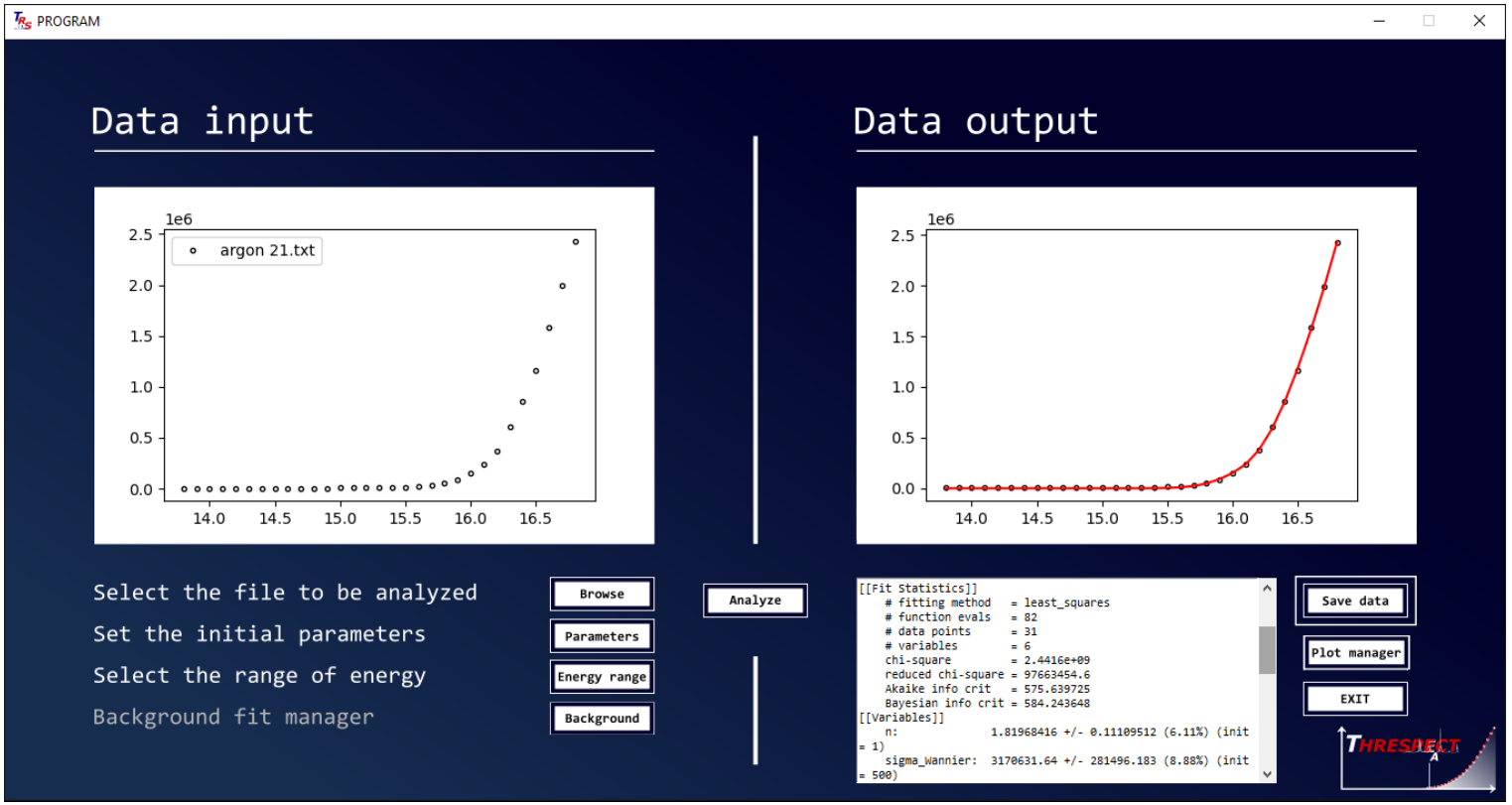
1) After starting the program, the file explorer should be used to select the file for analysis.
2) When loading the file, the range of values of the *x*-axis should be defined. The FWHM value of the incident beam should be entered in the next step. One can also set the initial values of all parameters.



3) Almost every cross-section experimental curve has some background that can be approximated by fitting a straight line. The software enables the determination of the parameters

a and *b* of such a line.

4) The program automatically saves all the parameters of the fitted curve in the file called "auto save.txt." This file is created automatically in the folder in which the program is located. After each run of the functions, the program will add new data below the previous ones. One can also save data in a file via the file explorer in a text file and a graph in the extensions "png" and "SVG."



In the figure, we present the output data of the example simulation.

EXAMPLES OF APPLICATION

Threshold energies were generated and compared to experimental spectra of many products measured using different experimental techniques to test the accuracy of predictions. Illustrative examples of our program applications using the fit procedure described above to cross-sections are only presented here. The figure shows the cross-section curves (open circles) and the corresponding fits (solid red lines) for two cations. In Table, the threshold energies, E_A, of corresponding products investigated are listed. The spectroscopic values or the results from original works are also presented for comparison.

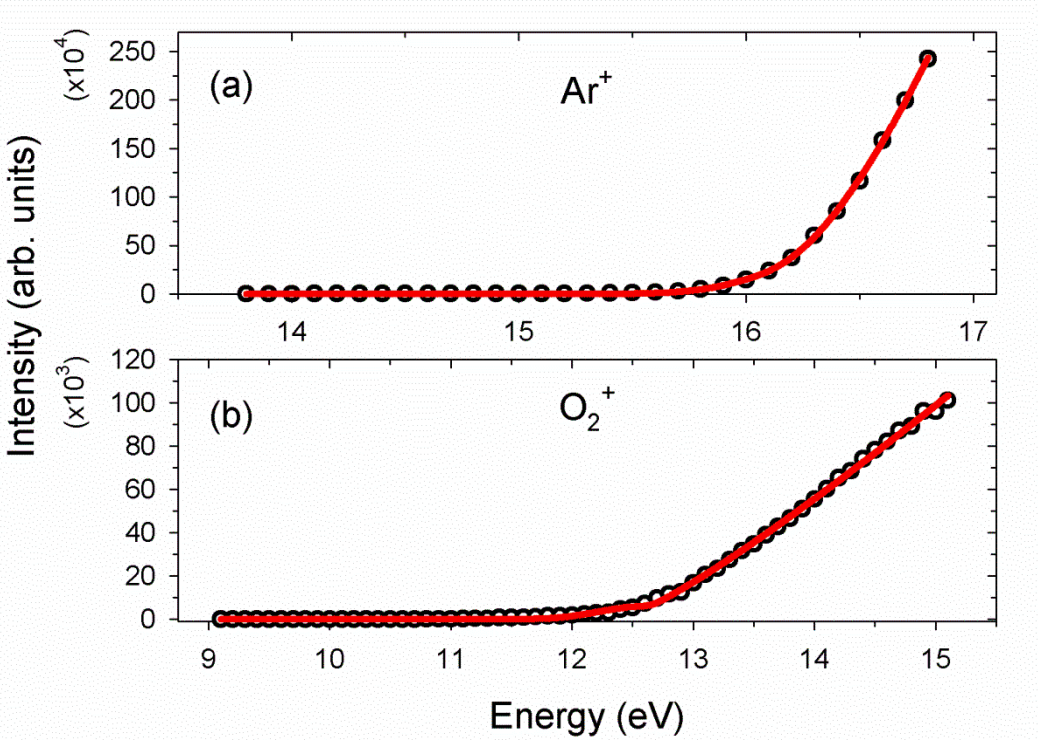


Table -Threshold energies, E_A, for the formation of different products compared with other spectroscopic appearance energies, E_{ASpec}. EIMS – electron impact mass spectrometry.

No.	Product/ technique	E_A [eV] this work	*n* this work	E_{ASpec} [eV]
(a)	Ar^+/ EIMS	15.9 (0.2)	1.4 (1.2)	15.76 (0.01) [1]
(b)	O_2^+/ EIMS	12.29 (0.09)	1.17 (0.03)	12.0696 (0.0003) [2]

SUMMARY

Here, we presented a computer program, "ThreSpect," enabling a fully automatic fitting procedure utilizing iterative non-linear optimization algorithms. By employing this program, we have simulated ample of the data measured by different spectroscopic techniques. Here we presented the program's functionality and only two examples of determining the threshold energies. The fittings allowed for a reliable statistical analysis of accumulated counts and gave excellent agreement between E_A obtained by us with values from other studies.

The computer program supporting this study's findings will soon be available in the MOST Wiedzy repository (https://mostwiedzy.pl/pl/open-research-data/catalog).

References

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2. R.G.Tonkyn, et al., Chem. Phys. Lett. **164**, 137-142 (1989).

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