Referee report of Tomáš Strapko doctoral thesis

ION SPECTROSCOPY FOR ANALYSIS OF SURFACE STRUCTURE

The thesis delt with fitting low enery ion scattering (LEIS) spectra. The author has introduced several possible fitting profiles and demonstrated their effects on experimental profiles. The author claims te

The thesis are relatively brief and are divided into three chapters. The first chapters describes basics of the LEIS and instrumentation. The second contains most results and the third chapter is called "Justification of L'Hoir peak, parameters of the fits and deconvolution formalism."

The author has presented approach to fit LEIS data and compared with modelling of multiple scattering and Monte Carlo TRBS simulations.

However, the presented work is not well organized. The theoretical sections are distributed all along the work. For example the deconvolution method results is shown in in section 2.2.5 and its mathematical background in section 3.3.5.

I have several questions and suggestions to the dissertation thesis:

- The fitting procedures are the main part of the thesis. However, no numerical results of the fitting parameters are shown or discussed except of peak intensity. It would be also great to discuss the peak positions and and width. How are these parameters affected by the fitting methods and what are their physical relevance? Especially, how does peak position
- The fitting of Gaussian and L'Hoir fit includes surface and binary collision peaks. What are difference of the surface peak and binary collision peak?
- The error function fit of the backgroud looks very similar to the Shirley type of background in XPS spectroscopy. What is the physical reason to intorduce shift of 30 eV between error function position and peak position?
- It would be great to include some overview of experimental data. There is a couple of spectra of Al foil at four primary energies in figure 1.11. The figure 2.29 and 2.30 suggests series of spectra taken at various primary energies for Al foil and Ag crystal. The CeO_2 is shown in a single graph and its fitting is not discussed at all. Data taken from silver crystal is shown only once and no its fitting at all.
- The deconvolution method needs and experimental resolution function. How was this function determined? What are the meaning of the various spectra shiown in deconvolution approach? Especially what is "deconvolution" and "background"?

- What is taken into integral in multiple scattering approach? Why is it so different from L'Hoir fit?
- On page 7, in formula (1.17) constant k is introduced. What does it mean?
- The claim about number of fitting parameters in part 2.2.1 is incorrect. The peak height and background intensity are also fitting parameters.
- How one can define FWHM of the error-function? Refers to part 3.3.1.

The thesis also includes couple of minor typos and inconsistencies. I want to mention few imperfections:

- on page 3 there is incorrect reference – words "Rik Ter Veen" except of actual reference.
- Page 5, top line typo in word screening.
- The thesis short overview on page 10 are missing reference.
- The formula 2.3 is definitely incorrect. The energy E is missing on the right side of equation.

T. Strapko reached the main goal to successfully fit the the data. The best results were obtained combining multiple scattering peaks with L'Hoir binary peak. The goals are highly relevant to the interpretation of LEIS spectroscopy. The input of doctorand has been clearly stated.

T. Strapko's doctoral thesis meets the required criteria. After answering he above questions I recommend to award T. Strapo with a title Ph.D.

Brno, 11. 11. 2024

doc. Ondřej Caha, Ph.D.