Application of MatLab for Processing X-ray Photoelectron Spectroscopy Spectra

Authors:
- Lubenchenco Aleksandr V.
- Ivanov Dmitry A.
- Lukyantsev Denis S.
National Research University "MPEI"

Speaker
Denis
Lukyantsev
National Research University "MPEI"
Relevance of Work

- currently, ultrathin films with a thickness of 3-10 nm are used in cryogenic electronics devices. In particular, the HEB-mixer (hot electron bolometer mixer or a mixer on the effect of electronic heating in superconducting films);

- niobium in contact with the environment is subject to oxidation, and, as is known, niobium oxides have very low electrical conductivity and their presence has a significant impact on the performance of such devices. By production of such a device, it is necessary to have a full understanding of the composition and structure of its main part – the film.
About the XPS Method

In the present work, the film analysis was carried out by the non-destructive method of X-ray photoelectron spectroscopy (XPS), which is based on the phenomenon of photoemission using monochromatic X-ray radiation and on determination of the energy of electronic levels by measuring kinetic energies of photoelectrons.
Useful Features of the MatLab Environment

- simple syntax of the language;
- efficiency;
- large number of standard mathematical functions (for example, findpeaks) that simplify programming;
- creating a drop-down menu;
- use of graphics environment;
- additional use of mouse actions.
M-files-Functions

- ImportDataXPS – import the recorded spectrum into the program, call the `uigetfile` function;
- Find – identification of spectrum peaks with their designation in accordance with the Handbook of X-ray Photoelectron Spectroscopy, calling the `findpeaks` function (included in the Signal Processing Toolbox);
- QuantChemAnalysis – quantitative chemical analysis;
M-files-functions

- Add_Reg – creation of a region;
- GetPoint – determination of the boundaries of the region;
- GetInterval – dividing the spectrum in this region into elementary points for further calculation;
- LineMove – changing the boundaries of the region;
- DeleteInterval – delete regions;
- DeletePoints – delete points.
Background Subtraction Methods and their M-functions

- **Shirley** (M-function Shirley): mathematical method;

- **Shirley–Proctor–Sherwood** (M-functions ShirleyProctorSherwood): takes into account the peaks of the previous multiple inelastically scattered photoelectrons in contrast to the usual Shirley mathematical method;

- **Tougaard** (M-functions Tougaard): follows from an approximate solution of the problem of multiple inelastic scattering of electrons in a solid.
Shirley–Proctor–Sherwood Method

\[ B_{SS,1}(E_K) = k_{SS,1} \int_{E_K}^{E_{K,\text{right}}} dE'_K \left[ I(E'_K) - I_{\text{right}} \right], \]

\[ B_{SS,2}(E_K) = k_{SS,2} \int_{E_K}^{E_{K,\text{right}}} dE'_K \left[ I(E'_K) - I_{\text{right}} - B_1(E'_K) \right], \]

\[ \ldots \]

\[ B_{SS,n}(E_K) = k_{SS,n} \int_{E_K}^{E_{K,\text{right}}} dE'_K \left[ I(E'_K) - I_{\text{right}} - B_{n-1}(E'_K) \right], \]

where \( B_{SS,n} \) is the \( n \)-th iteration in the SPS method,

\( E_K \) is the kinetic energy,

\( k_{SS,n} \) is the \( n \)-th iteration parameter of the SPS,

\( I(E_K) \) is the intensity of the photoelectric signal at \( E_K \).

\[ k_{SS,n} = \frac{I_{\text{left}} - I_{\text{right}}}{\int_{E_{K,\text{left}}}^{E_{K,\text{right}}} dE'_K \left[ I(E'_K) - I_{\text{right}} - B_{n-1}(E'_K) \right]} \]
Program Code in the Matlab Environment of the SPS Method

N=length(I);
BSS=zeros(1,N);
Iend = I(N);
I = I - I(N);
for n=1:itN
    kSS = I(1) / sum(I - BSS);
    for i=1:N
        BSS(i) = kSS*sum(I(i:N) - BSS(i:N));
    end
end
BSS = BSS + Iend;
Approximation Methods and Their M-functions

- **Gauss** – M-functions **Gauss1**: built-in function in MatLab;
- **Lorenz** – M-functions **Lorenz**: built-in function in MatLab;
- **Voigt** – M-functions **VoigtDS**: the sum of the Lorentzian and Gaussian. This function computes the complex scaled complementary error function also known as the FADDEEVA function:

\[
W_w(Z) = \exp(-Z^2) \times (1 - \text{erf}(-iZ)),
\]

Note that \(W_w(iX) = \text{erfcx}(X)\) for real-valued \(X\); \text{erfcx} is a build-in MatLab function.
Application of MatLab for Processing X-ray Photoelectron Spectroscopy Spectra

Survey Spectrum from a NbN Film on a Silicon Substrate

![Survey Spectrum from a NbN Film on a Silicon Substrate](image-url)

- N: 17.8%
- O: 39.7%
- Nb: 42.5%

Intensity (counts/s)

Binding Energy (eV)
Application of MatLab for Processing X-ray Photoelectron Spectroscopy Spectra

Detailed Spectrum of the Nb3d Line

![Graph](image-url)
Detailed Spectrum of the Nb 3d Line from a NbN Film
Detailed Spectrum of the O 1s Line from a NbN Film
There are functions that allow you to perform the following actions:

- reading experimental data of the X-ray photoelectron spectrum;
- automatic detection of photoelectron peaks;
- creating regions for each element;
- subtraction of the background by the linear method and the Shirley method;
- description of photoelectron peaks by approximation by the Gauss method.
Thank you for attention!

Speaker’s contacts:

Denis Lukyantsev
National Research University "MPEI"
LukyantsevDS@mpei.ru