Radiative transfer methods for electron spectroscopy

Pavel Kaplya[1], Viktor Afanas`ev, Dmitry Efremenko[2]
[1]National Research University «Moscow Power Engineering Institute», Krasnokazarmennaya 14, Moscow, Russia
[2]Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für Methodik der Fernerkundung (IMF), 82234 Oberpfaffenhofen, Germany

Synopsis Electron spectroscopy, invariant imbedding, XPS, PES, REELS

Reflected electron energy loss spectra (REELS) and X-Ray photoelectron spectroscopy (XPS) can be modeled by using the partial intensity approach (PIA), in which a spectrum is given by the weighted sum of multiple cross-convolutions of differential inverse inelastic mean free paths (DIIMFPs) and differential surface excitation probabilities. Computations of corresponding weights (partial intensities) is still a challenging task since the multiple scattering processes should be taken into account.

$$F(d,\Delta,\mu_0,\mu)=\sum_{k=0}^{\infty}F_k(d,\mu_0,\mu)x_{in}^k(\Delta). \qquad (1)$$

This work gives an overview of the numerical technique [1] recently proposed for computing partial intensities. It is based on the invariant imbedding method applied to the electron transport problem. It is shown that the partial intensities satisfy Riccati and Lyapunov equations, which are solved numerically in the discrete ordinate space by using the backward differential formula. The computed partial intensities are compared to those found by the straight line approximation, the small-angle approximation and the Oswald-Kasper-Gaukler model. The performance of the proposed method is significantly higher than that of Monte-Carlo methods with the similar accuracy.

The method is applied to computations of REELS and PES for a set of samples. A good agreement is obtained between simulated spectra and measurements. It is shown that a unified approach for REELS and PES gives a framework for extracting and validating DIIMFP data [2].

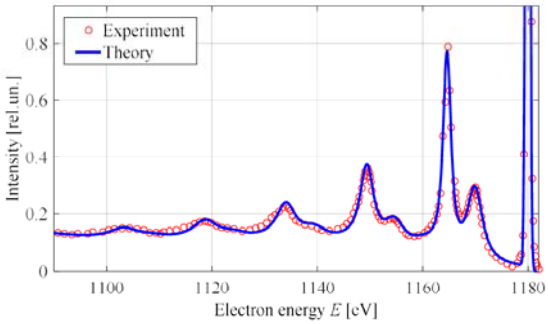

Figure 1. Comparison of experimental REELS spectra from Ref. [3] of Al with calculated spectra. The primary electron energies is 1180 eV; the average relative difference is 6.0%.

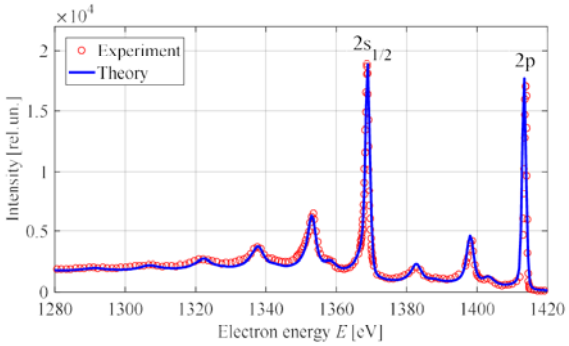

Figure 2. Comparison of the experimental PES spectrum [4] for Al. The average relative discrepancy is 7.8%.

References

1. V. Afanas`ev, D. Efremenko, P. Kaplya, JSERP **210** (2016) 16.
2. V. Afanas`ev, A. Gryazev, D. Efremenko, P. Kaplya, Vacuum. **136** (2017) 146.
3. S. Tougaard, I. Chorkendorff, Phys. Rev. B **35** (1987) 6570.
4. J. Moulder, et.al, Handbook of X-Ray Photoelectron Spectroscopy, 1995.

Email: pavel@kaplya.com