



Electron energy loss spectroscopy equation for spectra with overlapping oscillations and its solution by a regularization method



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ABSTRACT

The integral equation of EELFS spectra with the overlapping oscillations for two-component systems is proposed. To solve this equation Tikhonov's regularization method with the iterative procedure is applied. The atomic pair correlation functions of the investigated objects are obtained from the experimental EELFS spectra of $\text{Cu}_{50}\text{Ni}_{50}$ and $\text{Cu}_{50}\text{Mn}_{50}$ alloys by using Tikhonov's regularization method. The experimental results agree well with the known crystallographic data (partial interatomic distances, coordination numbers and Debye–Waller factors).

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1. Introduction

Electron spectroscopy is a traditional tool for analysis of the chemical composition of superthin (~ 1 nm) surface layers. The EELFS (Electron Energy Loss Fine Structure) method allows an analysis of the local atomic structure of surface layers 10–50 Å in thickness. The information on parameters of the local atomic structure from experimental EELFS spectra is contained in the partial atomic pair correlation functions (PCF). The EELFS spectra are formed by coherent scattering of the secondary electron on the local atomic environment and therefore, contain information about the local atomic structure of the substance. The EELFS spectra are signal intensity oscillations (with a period of 10–20 and a length up to 500 eV) localized on the low-energy side of the edges of energy losses [1]. The overlapping oscillations of EELF spectra are formed as a result of coherent scattering of secondary electrons on the local atomic environment from atom of one chemical grade or other. As a result, EELFS spectrum is a sum of two oscillations, determined by different wave numbers (p and q) that correspond to atoms of different chemical elements. The traditionally used Fourier transformation in case of overlapping oscillations [1–5] is not possible. The interval of overlapping oscillation in EELFS is defined by energy of the excited E_p and E_q levels, i.e. a rating of a nuclear environment (we will consider $E_p < E_q$). Thus, for processing EELFS spectrum of elements with a close values E_p and E_q excitement levels it is necessary to develop a new special technique.

In this paper, the mathematical model of EELFS spectra with overlapping oscillations is formed by an integral equation (or system of the integral equations). To solve the inverse problem of the definition of partial atomic pair correlation functions the Tikhonov's regularization method is used. The proposed method of the local atomic environment settings determination is tested on experimental EELFS spectra obtained from the surface of the test objects.

2. Mathematical model of overlapping EELFS oscillations

The intensity of the incident secondary electron whose coherent scattering by the local atomic environment of the excited atom forms the EELFS spectrum is recorded in the experiment. The information about atomic structure of the object is contained in the partial atomic pair correlation functions. For two-component systems with the atoms of types a and b the intensity of the EELFS spectrum may be written as:

$$J(E_p) = C_a J_a(E_p) \left[1 + 4\pi\rho_0 \int_0^\infty dr g_{aa}(r) \chi_{aa}(E_p, r) + 4\pi\rho_0 \int_0^\infty dr g_{ab}(r) \chi_{ab}(E_p, r) \right] + C_b J_b(E_q) \left[1 + 4\pi\rho_0 \int_0^\infty dr g_{ba}(r) \chi_{ba}(E_q, r) + 4\pi\rho_0 \int_0^\infty dr g_{bb}(r) \chi_{bb}(E_q, r) \right] \quad (1)$$

where C_a , C_b are concentrations of the elements a and b , ρ_0 is the atomic density of the sample, r is the distance between the excited atom and the neighboring atom, $g_{aa}(r)$, $g_{ab}(r) = g_{ba}(r)$ and $g_{bb}(r)$ are partial atomic pair correlation functions, J_a and J_b are intensities of excitation processes of internal levels of atoms of chemical elements a and b . The electron energies E_p and E_q (where p and q are

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the wave numbers) of the excited atoms of types *a* and *b* are defined:

$$E_p = \frac{\hbar^2}{2m} p^2, E_q = \frac{\hbar^2}{2m} q^2.$$

Interference terms are defined by the expressions:

$$\begin{aligned} \chi_{aa}(E_p, r) &= |\mu(E_p)| \frac{f_a(E_p)}{2p} \exp(-2r\gamma(E_p)) \cdot \sin(2pr + Q_a(E_p) + 2\delta_a(E_p)) \\ \chi_{ab}(E_p, r) &= |\mu(E_p)| \frac{f_b(E_q)}{2p} \exp(-2r\gamma(E_p)) \cdot \sin(2pr + Q_b(E_q) + 2\delta_a(E_p)) \\ \chi_{ba}(E_q, r) &= |\mu(E_q)| \frac{f_a(E_p)}{2q} \exp(-2r\gamma(E_q)) \cdot \sin(2qr + Q_a(E_p) + 2\delta_b(E_q)) \\ \chi_{bb}(E_q, r) &= |\mu(E_q)| \frac{f_b(E_q)}{2q} \exp(-2r\gamma(E_q)) \cdot \sin(2qr + Q_b(E_q) + 2\delta_b(E_q)) \end{aligned} \quad (2)$$

where γ^{-1} is the secondary electron mean free path; *f* is the amplitude of backscattering by the *j*-th atom, Q_a is the phase dispersion in the varieties of atom *a*, δ is the effective phase shift of elastic scattering on the excitable atom; $|\mu|$ is the angular correlation function. These parameters are named the parameters of elastic scattering of a secondary electron [6–8].

To obtain quantitative information on the parameters of the local atomic structure from experimental EELFS spectra the normalized oscillating part must be extracted. In this work to obtain normalized oscillating parts previously developed technique is used [8]. A priori information about the atomic structure parameters of elastic scattering of secondary electron (the scattering parameters – amplitude and phase of backscattering, partial phase shifts and others) is received from X-ray diffraction data by use of software package FFEF-7 [9]. The calculation of electron wave functions of core level of the atoms is performed by the use of works [10,11]. Thus, for two-component system with atoms of types *a* and *b* the normalized oscillating part may be extracted from the experimental EELFS spectra as follows:

$$\begin{aligned} \frac{C_a(J_a(E_p) - J_a^{(at)}(E_p)) + C_b(J_b(E_q) - J_b^{(at)}(E_q))}{C_a J_a^{(at)}(E_p) + C_b J_b^{(at)}(E_q)} = 4\pi\rho_0 \times \\ \int_0^\infty dr [A\chi_{aa}(E_p, r)g_{aa}(r) + (A\chi_{ab}(E_p, r) \\ + B\chi_{ba}(E_q, r))g_{ab}(r) + B\chi_{bb}(E_q, r)g_{bb}(r)] \end{aligned} \quad (3)$$

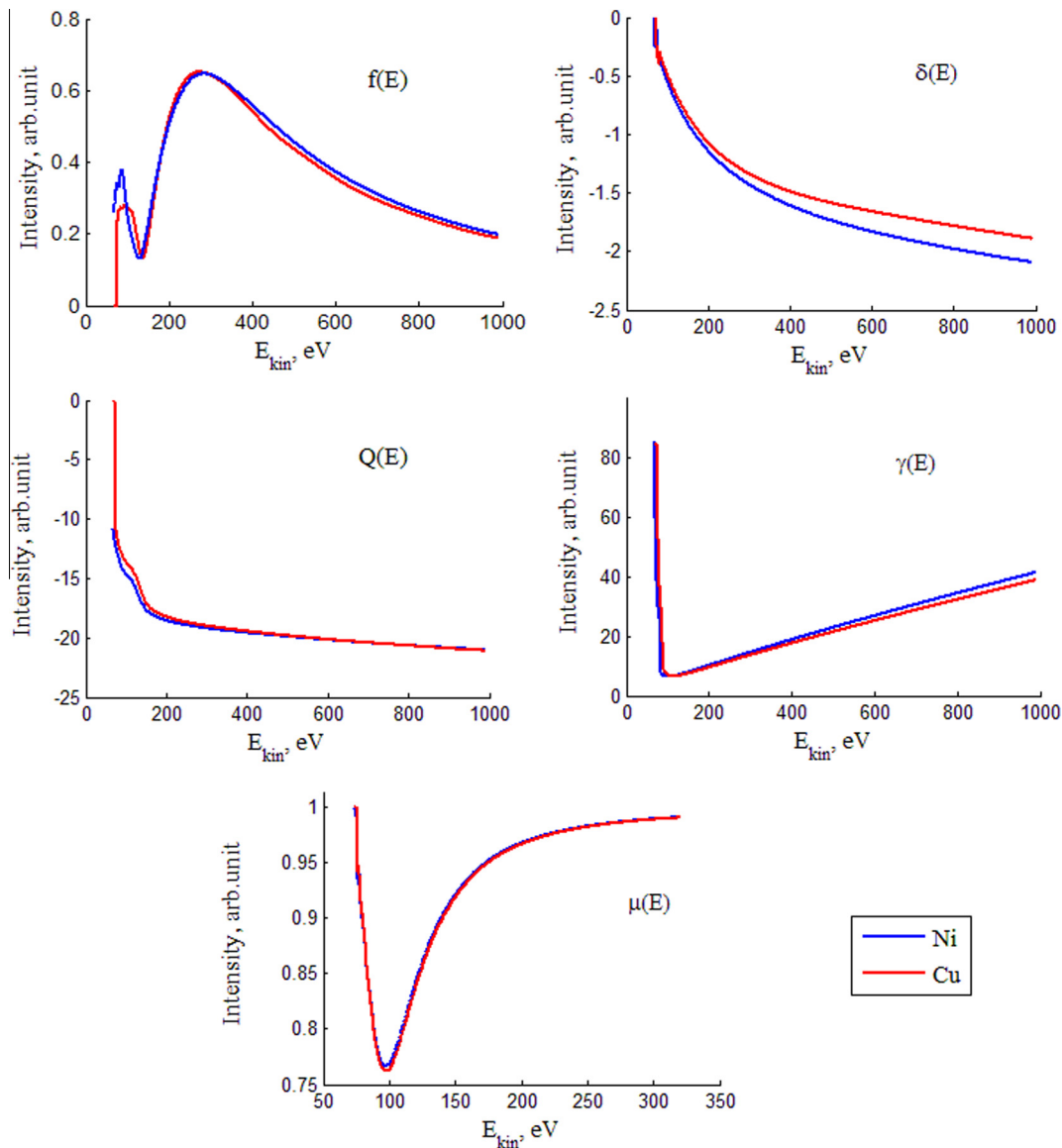


Fig. 1. The parameters of elastic scattering of a secondary electron.

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