Multipolarity effects in ionization of the inner level of an atom by an electron impact in extended fine structures of K and L spectra of electron energy losses

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Abstract

The problem of multipolarity of the atom core level ionization by electron impact in extended energy loss fine structure (EELFS) spectroscopy is studied. The intensities and amplitudes of electron transitions have been calculated in the OPW approximation. The experimental K EELFS spectra of Al, Si and L EELFS spectra of Fe, Co have been obtained. Corresponding calculations have been carried out in the monopole and dipole approximations. A comparison of theoretical and experimental spectra have been made. It is shown that a good agreement between the theoretical and experimental results points to the need for taking account of multipolarity of the electron transition processes in EELFS calculations.

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1. Introduction

The XAFS-like features in the electron energy loss spectra are observed on the low-energy side of the thresholds of energy loss spectra due to ionization of atom core levels by incident electrons. The extended energy loss fine structure (EELFS) is a result of coherent scattering of the secondary electron on the local atomic environment of the ionized atom [1,2]. Compared to XAFS [3], the EELFS method has a number of advantages:

– analysis of the local atomic structure of super-thin surface layers (in the range from 10 to 50 Å)
– a super high area resolution (down to several nanometers).

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However, to obtain reliable information about the local atomic configuration by the EELFS technique some aspects of the EELFS process must be worked out theoretically. Unlike the XAFS, the EELFS is more complicated since it forms as a result of the atom excitation by electron impact. So, the dipole selection rule specific for describing the XAFS process cannot be used in EELFS theory. In particular, theoretical description of the process of ionization of the core level by electron impact is a most serious problem, because, contrary to the radiation process forming the XAFS spectrum, in the EELFS mechanism the dipole rules do not work [4–9].

In the single scattering approximation the intensity of the incident electron energy loss due to ionization of the atom core level is determined as [10]

$$
\begin{aligned}
\mathrm{d}J(E_w - E_u) = \mathrm{d}J_{\mathrm{at}}(E_w - E_u)\Bigg[& 1 + Re \sum_l \mu_l (-1)^l \\
& \times \exp(i2\delta_l^0) W(T) f_j(p, \pi) \\
& \times \frac{\exp(i2p^+ R_j)}{ipR_j^2} \Bigg]
\end{aligned}
\tag{1}
$$

where $\mathrm{d}J_{\mathrm{at}}(E_w - E_u)$ is the intensity of the atomic process, $(E_w - E_u)$ is the incident electron energy loss. In Eq. (1) we use the following standard XAFS designations [3]: δ_1^0 are partial phase shifts of the ionized atom, $f_j(p, \pi)$ is the backscattering amplitude of the jth neighboring atom, $W(T)$ is the Debye–Waller factor, R_j is the interatomic distance; p is the secondary electron wave number defined from the energy conservation law $p^2 = w^2 - u^2 - 2E_\alpha$ (atomic units), and $p^+ = p + i/\lambda$, where λ is the mean free path of the secondary electron. In Eq. (1) summation is over all jth atoms. The multipolarity of the process of atom core level ionization by electron impact is determined by the coefficients μ_l, where

$$
\begin{aligned}
\sum_l \mu_l P_l(\cos \widehat{p, p_j}) &= \mu(\widehat{p, p_j}) \\
&= \frac{\langle T^*(p, \aleph) T(p_j, \aleph) \rangle}{\langle T^*(p, \aleph) T(p, \aleph) \rangle}
\end{aligned}
\tag{2}
$$

where P_l-Legendre polynomials. The correlation function $\mu(p, p_j)$ is determined by the averages

$\langle T^*(p, \aleph) T(p_j, \aleph) \rangle$ where $T^*(p, \aleph)$ and $T(p_j, \aleph)$ are the amplitudes of creation of the secondary electron wave with wave vectors p and $p_j(|p| = |p_j|)$, where $\aleph = w - u$ is the transferred momentum of the incident electron.

2. Comparison of the theoretical and experimental results

In the orthogonalized plane wave (OPW) approximation for the secondary electron wave function the amplitude of the atom core level ionization is

$$
\begin{aligned}
T_\alpha(p, \aleph) \sim \left(\frac{1}{\aleph^2} - \frac{1}{w^2}\right) \Bigg[& \langle p | \exp(i\aleph r) | \alpha \rangle \\
& - \sum_{|\alpha'\rangle} \langle p | \alpha' \rangle \langle \alpha' | \exp(i\aleph r) | \alpha \rangle \Bigg]
\end{aligned}
\tag{3}
$$

where $|p\rangle$ is a plane wave, $|\alpha\rangle$ is the wave function of the ionized atom core level, and $|\alpha'\rangle$ are all the atom core level wave functions. Eq. (3) is obtained with the condition $p^2/w^2 \ll 1$, which is usually a good approximation for EELFS spectroscopy.

The calculation of amplitudes (3) in spherical coordinates gives the averages that determine the correlation function $\mu(p, p_j)$ in the form

$$
\begin{aligned}
\langle T_\alpha^*(p, \aleph) T_\alpha(p_j, \aleph) \rangle \sim \left(\frac{1}{\aleph^2} - \frac{1}{w^2}\right)^2 (n_\alpha)^2 C_l^{l', l_\alpha} C_{l', l_\alpha}^l \\
\times |T_{\alpha l'}^l|^2 P_l(\cos \widehat{p, p_j}),
\end{aligned}
\tag{4}
$$

where C_{l', l_α}^l is the Gaunt integral. In Eq. (4) summation over all indices is implied.

To analyse the amplitudes and intensities of the atom core level ionization processes and calculate the corresponding EELFS spectra we shall take into account in Eq. (4) the effect of orthogonalization of the secondary electron wave function to K and $L_{2,3}$ core level wave functions in the case of ionization of the K core level, and to K, $L_{2,3}$ and $M_{4,5}$ in the case of ionization of the $L_{2,3}$ core level. In addition, we shall use the 1s-, 2p- and 3d-hydrogen like wave functions as K, $L_{2,3}M_{4,5}$ core level wave functions, respectively. In this approach, the averages (Eq. (2)) and the corresponding coefficients μ_l are calculated analytically. A