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*A*UGER-ELECTRON SPECTROSCOPY OF TRANSIENT METALS

The calculated data on the Auger-transition energies for a number of metals (Fe, Co, Cu, Zn) are presented and compared with theoretical data by the semi-empirical method by Larkins as well as experimental data. As basic approach to calculating the Auger spectra of solids we use a new approach, basing on the S-matrix formalism by Gell-Mann and Low and relativistic perturbation theory formalism.

This work goes on our investigation of the characteristics for the Auger effect in atomic systems and solids [1-7]. As introduction let us remind [1] that the Auger electron spectroscopy remains an effective method to study the solids electron structure, chemical composition of solid surfaces and near-surface layers [8-12]. Sensing the Auger spectra in atomic systems and solids gives the important data for the whole number of scientific and technological applications. So called two-step model is used most widely when calculating the Auger decay characteristics [8-13]. Since the vacancy lifetime in an inner atomic shell is rather long (about 10^{-17} to 10^{-14}s), the atom ionization and the Auger emission are considered to be two independent processes. In the more correct dynamic theory of the Auger effect [9] the processes are not believed to be independent from one another. The fact is taken into account that the relaxation processes due to Coulomb interaction between electrons and resulting in the electron distribution in the vacancy field have no time to be over prior to the transition. In fact, a consistent Auger decay theory has to take into account correctly a number of correlation effects, including the energy dependence of the vacancy mass operator, the continuum pressure, spreading of the initial state over a set of configurations etc.

Now it is clear that an account of the relativistic and exchange-correlation effects is very important for the adequate description of the Auger spectra of atoms and solids. This problem is partly solved in this paper. As basic approach to calculating the Auger spectra of solids we use a new approach [1-7], basing on the S-matrix formalism by Gell-Mann and Low and relativistic perturbation theory (PT) formalism [13]. Earlier the method has been applied to calculation of the Auger-electron spectra (transitions), the ionization cross-sections of inner shells in various atomic systems and solids [1-7]. In this paper we apply this method to studying the Auger –electron parameters fro a number for a number of the transient metals.

As the key aspects of our approach have been earlier described [1-7], here we are limited by a brief consideration. Within the frame of the relativistic many-body theory , the Auger transition probability and the Auger line intensity are defined by the square of an electron interaction matrix element having the form:

$$V^{\omega}_{1234} = [(j_1)(j_2)(j_3)(j_4)]^{1/2} \sum_{\lambda\mu} (-1)^{\mu} \begin{pmatrix} j_1 j_3 & \lambda \\ m_1 - m_3 & \mu \end{pmatrix} \cdot \\ \cdot \operatorname{Re} Q_{\lambda}(1234)$$

$$Q_{\lambda} = Q_{\lambda}^{\mathrm{Qul}} + Q_{\lambda}^{\mathrm{Br}} . \qquad (1)$$

The terms $Q_{\lambda}^{\mathrm{Qul}}$ and Q_{λ}^{B} correspond to subdivision of the potential into Coulomb part $cos|w|r_{12}/r_{12}$ and Breat one, $cos|w|r_{12}\boldsymbol{a_1}\boldsymbol{a_2}/r_{12}$. The real part of the electron interaction matrix element is determined using expansion in terms of Bessel functions:

$$\frac{\cos|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}} \sum_{\lambda=0} (\lambda) J_{\lambda+1/2}(|\omega|r_<) \\ J_{-\lambda-1/2}(|\omega|r_>) P_{\lambda}(\cos \mathbf{r}_1 \mathbf{r}_2) \qquad (2)$$

where J is the 1st order Bessel function, (l)=2l+1.

The Coulomb part Q_λ^{Qul} is expressed in terms of the radial integrals R_1 and the angular coefficients S_1 [13]:

$$\begin{aligned}\mathrm{Re}\,Q_\lambda^{\mathrm{Qul}} = \frac{1}{Z}\,\mathrm{Re}\{R_l(1243)S_\lambda(1243)+ + \\ + R_\lambda(\tilde{1}24\tilde{3})S_\lambda(\tilde{1}24\tilde{3})+ \\ + R_\lambda(1\tilde{2}\tilde{4}3)S_\lambda(1\tilde{2}\tilde{4}3)+ R_\lambda(\tilde{1}\tilde{2}43)S_\lambda(\tilde{1}\tilde{2}43)\}\end{aligned} \tag{3}$$

As a result, the Auger decay probability is expressed in terms of $\mathrm{Re}Q_1(1243)$ matrix elements:

$$\begin{aligned}\mathrm{Re}\,R_\lambda(1243) = \iint dr_1 r_1^2 r_2^2 f_1(r_1) f_3(r_1).\\ f_2(r_2) f_4(r_2) Z_\lambda^{(1)}(r_<) Z_\lambda^{(1)}(r_>)\end{aligned} \tag{4}$$

where f is the large component of radial part of single electron state Dirac function; function Z and angular coefficient are defined in refs. [2-4,13]. The other items in (3) include small components of the Dirac functions; the sign «~» means that in (3) the large radial component f_i is to be changed by the small g_i one and the moment l_i is to be changed by $\tilde{l}_i = l_i - 1$ for Dirac number æ$_1$> 0 and l_i+1 for æ$_i$<0.

The Breit interaction is known to change considerably the Auger decay dynamics in some cases. The Breit part of Q is defined in [7,13]. The Auger width is obtained from the adiabatic Gell-Mann and Low formula for the energy shift [7]. Namely, according to [1,7], the Auger level width with a vacancy $n_a l_a j_a m_a$ can be represented as:

$$\sum_\lambda \frac{2}{(\lambda)(j_\alpha)} \sum_{\beta\gamma\le f\, k>f} \sum Q_\lambda(\alpha k\gamma\beta) Q_\lambda(\beta\gamma k\alpha) \quad , \tag{5}$$

$$\frac{2}{(j_\alpha)} \sum_{\lambda_1\lambda_2} \sum_{\beta\gamma\le f\, k>f} \sum Q_{\lambda_1}(\alpha k\gamma\beta) Q_{\lambda_2}(\beta\gamma k\alpha) \begin{Bmatrix} j_\alpha & j_\gamma & \lambda_2 \\ j_k & j_\beta & \lambda_1 \end{Bmatrix} \tag{6}$$

The partial items of the $\sum_{\beta} \sum_{k}$ sum answer to contributions of a^{-1}®(bg)^{-1}K channels resulting in formation of two new vacancies bg and one free electron k: w_k=w_a+w_b–w_a. The final expression for the width in the representation of jj-coupling scheme of single-electron moments is given by the corresponding sum on over all possible decay channels.

The basis of the electron state functions was determined by the solution of Dirac equation (integrated numerically using the Runge-Cutt method). The contribution of the lower order PT corrections to the energies of the auger transitions is carried out according to the methodology [11,12,14]. The calculation of radial integrals **Re**R_1(1243) is reduced to the solution of a system of differential equations [13]:

$$\begin{aligned} y_1' &= f_1 f_3 Z_\lambda^{(1)}(\alpha|\omega|r) r^{2+\lambda} \\ y_2' &= f_2 f_4 Z_\lambda^{(1)}(\alpha|\omega|r) r^{2+\lambda} \\ y_3' &= [y_1 f_2 f_4 + y_2 f_1 f_3] Z_\lambda^{(2)}(\alpha|\omega|r) r^{1-\lambda} \end{aligned} \tag{7}$$

In addition,$y_3(\infty)$=**Re**R_1(1243), y_1(¥)=X_1(13). The formulas for the Auger decay probability include the radial integrals R_a(a$k$gb), where one of the functions describes electron in the continuum state.

The energy of an electron formed due to a transition jkl is defined by the difference between energies of atom with a hole at j level and double-ionized atom at kl levels in final state:

$$E_A(jkl, {}^{2S+1}L_J) = E_A^+(j) - E_A^{2+}(kl, {}^{2S+1}L_J) \tag{8}$$

In order to take into account the dynamic correlation effects, the equation (8) can be rewritten as:

$$E_A(jkl, {}^{2S+1}L_J) = E(j) - E(k) - E(l) - \Delta(k,l; {}^{2S+1}L_J) \tag{9}$$

where the item D takes into account the dynamic correlation effects (relaxation due to hole screening with electrons etc.) To take these effects into account, the set of procedures elaborated in the atomic theory [2,3] is used. For solid phase, the more precise form of equation (9) is as follows:

$$E^s A(jkl, {}^{2S+1}L_J) = E_A(jkl, {}^{2S+1}L_J) + \Delta E^s + R_{rel} + e\Phi \tag{10}$$

where DE^s is a correction for the binding energy change in the solid; R_{rel}, the same for out-of-atom relaxation; eF takes into account the work of output. Other details can be found in Refs. [1-7].

In table 1 we present our calculation data on Auger-electron energies (column B) and also the semi-empirical method under Larkins' equivalent core approximation (from [8,9] (column A) as well as experimental data [2].

The calculation accuracy using the Larkins' method is within about 2 eV as an average. Our approach provides more accurate results that is due to a considerable extent to more correct accounting for the exchange-correlation effects.

Table 1. **Experimental and theoretical data for Auger electron energy: Exp-experiment; A, semi-empirical method - [8,9]; B- present paper;**

Solid	Auger line	Exp	Theory: A	Theory: D
Fe	$L_3M_{4,5}M_{4,5}\ ^1G_4$	701.2	702.8	701.3
Co	$L_3M_{4,5}M_{4,5}\ ^1G_4$	772.5	772.8	772.7
Cu	$L_3N_{4,5}N_{4,5}\ ^1G_4$	919.0	922.5	919.1
Zn	$L_3N_{4,5}N_{4,5}\ ^1G_4$	991.8	994.0	991.8

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Abstract

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Key words: Auger-transitions, transient metals

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ОЖЕ-ЭЛЕКТРОННАЯ СПЕКТРОСКОПИЯ ПЕРЕХОДНЫХ МЕТАЛЛОВ

Резюме

Приведены результаты расчета энергий Оже-переходов для ряда металлов (Fe, Co, Cu, Zn) и проведено их сравнение с теоретическими данными, полученными на основе полуэмпирического метода с Ларкинса , а также экспериментальными данными. Для расчета параметров Оже-спектров твердых тел использован новый подход, который базируется на S-матричном формализме Гелл-Манна и Лоу и формализме релятивистской теории возмущений.

Ключевые слова: Оже-переходы, переходные металлы

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ОЖЕ-ЕЛЕКТРОННА СПЕКТРОСКОПІЯ ПЕРЕХІДНИХ МЕТАЛІВ

Резюме

Наведені результати розрахунку енергій Оже-переходів для ряду металів (Fe, Co, Cu, Zn) та проведено їх порівняння з теоретичними даними, отриманими на основі напівемпіричного методу Ларкінса, а також експериментальними даними. Для розрахунку параметрів Оже-спектрів твердих тіл використаний новий підхід, який базується на S-матричному формалізмі Гелл-Манна і Лоу і формалізмі релятивістської теорії збурень.

Ключові слова: Оже-переходи, перехідні метали