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CALCULATION OF AUGER-ELECTRON ENERGIES FOR SOME SOLIDS

Within a new relativistic approach there are presented the calculation data on the Auger electron transition energies for solids of As and Ag. New data on the Auger-electron energies for atoms and solids of the As and Ag are analyzed and compared with alternative theoretical semiempirical equivalent core approximation results, obtained by Larkins as well as experimental data. There is physically reasonable agreement between theory and experiment.

I. Introduction

This work goes on our investigation in a field of theoretical Auger spectroscopy of atoms and solids [1,2]. In Refs. [1-7] there were presented the calculation data on the Auger electron transition energies for a whole number of atomic systems and solids, in particular, alkali and transient metals and inert gases. Here we present the Auger electron energy data for As and Ag.

In eRefs. [1,2] it has been indicated that the Auger electron spectroscopy remains an effective method to study the solids electron structure, chemical composition of solid surfaces and nearsurface 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 [8-14]. 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]. Here we are limited only by the key topics. Other details can be, for example, found in Refs. [1-5].

2. Method

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:

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

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

The terms QQ_{λ}^{Qul} and Q correspond to subdivision of the potential into Coulomb part

cos\rn\$r_{I2}$/$r_{I2}$ and Breat one, *cos\rn\$r_{I2}a_Ia_2$/$r_{I2}$*. The real part of the electron interaction matrix element is determined using expansion in terms of Bessel functions:

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

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

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

$$\mathrm{Re}Q_\lambda^{Qul} = \frac{1}{Z}\mathrm{Re}\{R_l(1243)S_\lambda(1243) + R_\lambda(\tilde{1}24\tilde{3})S_\lambda(\tilde{1}24\tilde{3}) + \quad (3)$$

$$+ R_\lambda(1\tilde{2}\tilde{4}3)S_\lambda(1\tilde{2}\tilde{4}3) + R_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3})S_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3})\}$$

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

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

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 l_1. is to be changed by the small g_1 one and the moment l_1 is to be changed by $\tilde{l}_i = l_i - 1$ for Dirac number $æ_1 > 0$ and $l_i - 1$ for $æ_1 < 0$.

The Breit interaction is known to change considerably the Aug er dec ay 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 $n_\alpha l_\alpha j_\alpha m_\alpha$ can be re presented as:

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

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

The partial item s of the $\sum_{\beta\gamma}\sum_k$ sum answer to contributions of $\alpha^{-1}\rightarrow(\beta\gamma)^{-1}K$ channels resulting in formation of two new vacancies $\beta\gamma$ and one free electron k: $\omega_k=\omega_\alpha+\omega_\beta-\omega_\alpha$. 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 transition s is carried out according to the methodology [11,12,14]. The calculation of radial integrals $\mathbf{Re}R_\lambda(1243)$ is reduced to the solution of a system of differential equations [13]:

$$y_1' = f_1 f_3 Z_\lambda^{(1)}(\alpha|\omega|r) r^{2+\lambda}$$

$$y_2' = f_2 f_4 Z_\lambda^{(1)}(\alpha|\omega|r) r^{2+\lambda} \quad (7)$$

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

In addition,
$y_3(\infty)=\mathbf{Re}R_\lambda(1243)$,
$y_1(\infty)=X_\lambda(13)$.

The formulas for the; Aug er decay probability include the radial integrals $R_\alpha(\alpha k\gamma\beta)$, where one of the function s descri bes de ctron 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:

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

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

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

where the item A 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:

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

Where ΔE^s is a correction for the binding energy change in the solid; R_{rel} the same for out-of-atom relaxation; $e\Phi$ takes into account the work of output. Other details can be found in Refs. [1-7].

3. Some results

In table 1 we present our calculation data on Auger-electron energies for As and Ag (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 2a few V as an average. As earlier calculation show, our approach provides more accurate results that is due to a considerable extent to more correct accounting for the exchange-cor- relation effects. Especially physically reasonable accuracy has reached for alkali and alkali-earth elements. At the same time atoms of the transient metals are related to significantly more complex systems and a role of different exchange-correlation effects is of a critical importance. However, we believe that an approach used can be improved at this case too.

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
As	$L_3M_{4,5}M_{4,5}$ $^1G_4$	1226,4	1227,1	1226,6
Ag	$M_5N_{4,5}N_{4,5}$ $^1G_4$	353.4	358.8	354.8

References

1. Nikola L.V., Ignatenko A.V., Shakhman A.N., Relativistic theory of Auger (auto-ionization) decay of excited states in spectrum of multicharged ion// Photo-electronics.- 2010.-N19.-P.61-64.
2. Nikola L.V., Resonant Auger spectroscopy of the atoms of inert gases //Pho- to-electronics.-2011.-Vol.20.-P. 104-108.
3. Svinarenko A.A., Nikola L.V., Prepelitsa G.P., Tkach T., Mischenko E., The Auger (autoionization) decay of excited states in spectra of multicharged ions: Relativistic theory//Spectral Lines Shape (AIP,USA).-2010.-Vol.l6.-P94-98.
4. Ambrosov S.V., Glushkov A.V., Nikola L.V., Sensing the Auger spectra for solids: New quantum approach// Sensor Electr. and Microsyst. Techn.-2006.- N3.-P.46-50.
5. Nikola L.V., Quantum calculation of Auger spectra for Na, Si atoms and solids//Photoelectronics.-2007.-N16.- P.102-105.
6. Khetselius O.Yu., Nikola L.V., Turin A.V., Sukharev D.E., Sensing the finite size nuclear effect in calculation of the Auger spectra for atoms and solids// Sensor Electr. and Microsyst. Techn.-2007.-N1.-P.18-21..
7. Glushkov A.V., Khetselius O.Yu., Nikola L.V., Dubrovskaya Yu.V., Quantum calculation of Auger spectra for atoms and semiconductors: New approach// Photoelectronics.-2008.-N17.-P. 12-16.
8. Nikola L.V., Auger-electron spectroscopy of transient metals// "Photoelectronics" - 2013.-Vol.22.-P. 135-138
9. Aberg T., Hewat G. Theory of Auger effect. Springer-Verlag: Berlin, 1999.
10. Amusia M.Ya. Atomic photoeffect. Acad.Press: N.-Y., 1998.
11. Letokhov V. Nonlinear Selective Pho-toprocesses in Atoms and Molecules.- Moscow, 1997.
12. Aglitsky E.V., Safronova U.I. Spectroscopy of Autoionization states of atomic systems. Energoatomizd.: Moscow, 1992.
13. Glushkov A.V., Relativistic Quantum Theory. Quantum Mechanics of Atomic Systems.-Odessa: Astroprint, 2008.704p.
14. Kulekshov V.F., Kukharenko Yu.A., Fridrikhov S.A. et al. Spectroscopy and Electron Diffraction in Solid Surfaces Studies. Nauka: Moscow, 1995.

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Key **words:** Auger-spectroscopy, atoms, solids

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РАСЧЕТ ЭНЕРГИЙ ОЖЕ-ЭЛЕКТРОНОВ ДЛЯ ТВЕРДЫХ ТЕЛ

Резюме

В рамках нового релятивистского подхода выполнен расчет энергий Оже переходов для ряда твердых тел. Новые данные по Оже-электронным энергиям для As и Ag анализируются и сравниваются с альтернативными теоретическими полуэмпирическими данными, полученными в приближении эквивалентного остова Larkins, а также экспериментальными результатами.. Получено достаточно хорошее согласие теории и эксперимента.

Ключевые слова: Оже-спектроскопия, атомы, твердые тела

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РОЗРАХУНОК ЕНЕРГІЙ ОЖЕ ЕЛЕКТРОНІВ ДЛЯ ТВЕРДИХ ТІЛ

Резюме

В межах нового релятивістського підходу виконано розрахунок енергій Оже переходів для ряду твердих тіл. Нові дані по Оже-електронним енергіям для As і Ag аналізуються і порівнюються з альтернативними теоретичними напівемпіричними даними, отриманими у наближенні еквівалентного остову Larkins а також експериментальними результатами. Получено достатньо добре узгодження теорії та експерименту..

Ключові слова: Оже-спектроскопія, атоми, тверді тела