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THEORETICAL AUGER SPECTROSCOPY OF SOLIDS: CALCULATION OF ENERGY PARAMETERS

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Abstract. The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order density functional approximation is applied to determination of the energy and spectral parameters of the Auger decay for the Na, Si, Ge, Ag solids. The results are compared with reported experimental results as well as with those obtained by alternative theoretical schemes. The important point is linked with an accurate accounting for the complex exchange-correlation (polarization) effect contributions and using the optimized one-quasiparticle representation in the zeroth approximation of relativistic many-body perturbation theory, which significantly affects the agreement of theory and experiment.

Keywords: relativistic theory, Auger spectroscopy, solids

ТЕОРЕТИЧНА ОЖЕ-СПЕКТРОСКОПІЯ ТВЕРДОГО ТІЛА: РОЗРАХУНОК ЕНЕРГЕТИЧНИХ ПАРАМЕТРІВ

О. В. Глушков, В. В. Буйаджи, А. В. Цудик, О. С. Чернишев, Е. О. Єфімова

Анотація. Комбінований релятивістський енергетичний підхід і релятивістська багаточастинкова теорія збурень з нульовим наближенням функціонала густини застосовуються для визначення енергетичних і спектральних параметрів Оже-процесу в твердотільних Na, Si, Ge, Ag. Результати порівнюються з узагальненими експериментальними даними, а також з результатами, отриманими на основі альтернативних теоретичних методів. Важливий момент пов'язаний з урахуванням вкладів складних багаточастинкових обмінно-кореляційних ефектів та використанням оптимізованого одночастинкового уявлення в нульовому наближенні релятивістської багаточастинкової теорії збурень, що суттєво впливає на згоду теорії та експерименту.

Ключові слова: релятивістська теорія, Оже-спектроскопія, тверде тіло

ТЕОРЕТИЧЕСКАЯ ОЖЕ-СПЕКТРОСКОПИЯ ТВЕРДОГО ТЕЛА: РАСЧЕТ ЭНЕРГЕТИЧЕСКИХ ПАРАМЕТРОВ

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Аннотация. Комбинированный релятивистский энергетический подход и релятивистская многочастичная теория возмущений с приближением функционала плотности нулевого порядка применяются для определения энергетических и спектральных параметров оже-процесса в твердотельных Na, Si, Ge, Ag. Результаты сравниваются с обобщенными экспериментальными результатами, а также с результатами, полученными в рамках альтернативных теоретических подходов. Важный момент связан с учетом вкладов многочастичных корреляционных эффектов и использованием оптимизированного одночастичного представления в нулевом приближении многочастичной теории возмущений, что существенно влияет на согласие теории и эксперимента.

Ключевые слова: релятивистская теория, Оже-спектроскопия, твердое тело

Introduction

The Auger electron spectroscopy is an effective method to study the chemical composition of solid surfaces and near-surface layers etc [1-8]. Sensing the Auger spectra in atomic systems and solids gives the important data for the whole number of scientific and technological applications. When considering the method principles, the main attention is given as a rule to the models for drawing chemical information from the Auger spectra and to the surface composition determination methods by the Auger spectrum decoding. It is just the two-step model that is used most widely when calculating the Auger decay characteristics. 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 [1-4] 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. [9-20]. Note that

the effects are not described adequately to date, in particular within the Auger decay theory [2].

The most widespread theoretical studying the Auger spectra parameters is based on using the multi-configuration Dirac-Fock (MCDF) calculation [1-3]. The theoretical predictions based on MCDF calculations have been carried out within different approximations and remained hitherto non-satisfactory in many relations. Earlier [11,12] it has been proposed relativistic perturbation theory (PT) method of the Auger decay characteristics for complex atoms, which is based on the Gell-Mann and Low S-matrix formalism energy approach and many-body perturbation theory (PT) formalism [4-7]. The novel element was in using the optimal basis of the electron state functions derived from the minimization condition for the calibration-non-invariant contribution (the second order PT polarization diagrams contribution) to the imaginary part of the multi-electron system energy already at the first non-disappearing approximation of the PT. Earlier it has been applied in studying the Auger decay characteristics for a set of neutral atoms and quasi-molecules. Besides, the ionization cross-sections of inner shells in various atoms and the Auger electron energies in solids were estimated. In this paper the combined relativistic energy approach and relativistic many-body PT with the zeroth order density functional approximation is used for sensing the Auger spectra of solids and calculation of their energy parameters.

The theoretical method

In Refs. [4,5,16-22] the fundamentals of the relativistic many-body PT formalism have been in detail presented, so further we are limited only by the novel elements. Let us remind that the majority of complex atomic systems possess a dense energy spectrum of interacting states. In Refs. [1, 3-5] there is realized a field procedure for calculating the energy shifts ΔE of degenerate states, which is connected with the secular matrix M diagonalization. The whole calculation of the energies and decay probabilities of a non-degenerate excited state is reduced to the calculation and diagonalization of the complex secular matrix. In the relativistic energy approach [4-9], which has received a great applications during solving numerous problems of atomic, molecular and nuclear physics (e.g., see Refs. [1, 4, 5, 23-30]), the imaginary part of electron energy shift of an atom is directly connected with the radiation decay possibility (transition probability). An approach, using the Gell-Mann and Low formula with the QED scattering matrix, is used in treating the relativistic atom. The total energy shift of the state is usually presented in the form:

$$\Delta E = \text{Re} \Delta E + i \Gamma / 2, \tag{1}$$

where Γ is interpreted as the level width, and the decay possibility $P = \Gamma$. The imaginary part of electron energy of the system, which is defined in the lowest order of perturbation theory as [4]:

$$\text{Im} \Delta E(B) = -\frac{e^2}{4\pi} \sum_{\substack{\alpha > n > f \\ [\alpha < n \leq f]}} V_{\alpha n \alpha n}^{|\omega_{\alpha n}|}, \tag{2}$$

where $(\alpha > n > f)$ for electron and $(\alpha > n > f)$ for vacancy; $V_{\alpha n \alpha n}^{|\omega_{\alpha n}|}$ is an imaginary part of the matrix element of the potential:

$$V(r_i r_j) = \exp(i\omega r_{ij}) \cdot \frac{(1 - \alpha_i \alpha_j)}{r_{ij}}. \tag{3}$$

Within the frame of the relativistic PT approach the Auger transition probability and the Auger line intensity are defined by the square of an electron interaction matrix element having the form [2-4]:

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

$$Q_{\lambda} = Q_{\lambda}^{\text{Qu}} + Q_{\lambda}^{\text{Br}}. \tag{5}$$

The terms Q_{λ}^{Qu} and Q_{λ}^{Br} correspond to subdivision of the potential into Coulomb part $\cos|\omega|r_{12} a_1 a_2 / r_{12}$. The real part of the electron interaction matrix element is determined using expansion in terms of Bessel functions:

$$\frac{\cos|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}} \sum_{\lambda=0} (\lambda) J_{\lambda+1/2}(|\omega|r_{<}) J_{-\lambda-1/2}(|\omega|r_{>}) P_{\lambda}(\cos \mathbf{r}_1 \mathbf{r}_2) \tag{6}$$

where J is the 1st order Bessel function, $(\lambda) = 2\lambda + 1$. The Coulomb part Q_{λ}^{Qu} is expressed in terms of radial integrals R_l angular coefficients S_l according to Refs [4]. The Breat interaction is known to change considerably the Auger decay dynamics in some cases. The Breat part of Q is defined in [2-4].

The Auger width is obtained from the adiabatic Gell-Mann and Low formula for the energy shift [3]. The direct contribution to the Auger level width with a vacancy $n_a l j_a m_a$ is as follows:

$$\sum_{\lambda} \frac{2}{(\lambda)(j_a)} \sum_{\beta \gamma \leq f} \sum_{k > f} Q_{\lambda}(ak\gamma\beta) Q_{\lambda}(\gamma\beta k\alpha), \tag{7}$$

while the exchange diagram contribution is:

$$\frac{2}{(j_a)} \sum_{\lambda_1 \lambda_2} \sum_{\beta \gamma \leq f} \sum_{k > f} Q_{\lambda_1}(ak\gamma\beta) Q_{\lambda_2}(\gamma\beta k\alpha) \begin{Bmatrix} j_a & j_{\gamma} & \lambda_2 \\ j_k & j_{\beta} & \lambda_1 \end{Bmatrix} \tag{8}$$

The partial items of the $\sum_{\beta \gamma} \sum_k$ sum answer to contributions of $a^{-1} \rightarrow (\beta \gamma)^{-1} K$ channels resulting in formation of two new vacancies $\beta \gamma$ and one free electron k : $\omega_k = \omega_{\alpha} + \omega_{\beta} + \omega_{\alpha}$. The calculating of all matrix elements, wave functions, Bessel functions etc is reduced to solving the system of differential equations. The formulas for the autoionization (Auger) decay probability include the radial integrals $R_a(ak\gamma\beta)$, where one of the functions describes electron in the continuum state. When calculating this integral, the correct normalization of the wave functions is very im-

portant, namely, they should have the following asymptotic at $r \rightarrow 0$:

$$\left. \begin{matrix} f \\ g \end{matrix} \right\} \rightarrow (\lambda\omega)^{-1/2} \begin{cases} [\omega + (\alpha Z)^{-2}]^{-1/2} \sin(kr + \delta), \\ [\omega - (\alpha Z)^{-2}]^{-1/2} \cos(kr + \delta). \end{cases} \quad (9)$$

The important aspect of the whole procedure is an accurate accounting for the exchange-correlation effects. We have used the generalized relativistic Kohn-Sham density functional [3-5] in the zeroth approximation of relativistic PT; naturally, the perturbation operator contents the operator (7) minus the cited Kohn-Sham density functional. Further the wave functions are corrected by accounting of the first order PT contribution. Besides, we realize the procedure of optimization of relativistic orbitals base. The main idea is based on using ab initio optimization procedure, which is reduced to minimization of the gauge dependent multielectron contribution $Im\Delta E_{ninv}$ of the lowest QED PT corrections to the radiation widths of atomic levels.

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:

$$E_A(jkl, 2^{S+1}L_J) = E_A^+(j) - E_A^{2+}(kl, 2^{S+1}L_J). \quad (10)$$

In the solids theory, to single out the important correlation and medium effects, the equation (10) is usually rewritten as:

$$E_A(jkl, 2^{S+1}L_J) = E(j) - E(k) - E(l) - \Delta(k, l, 2^{S+1}L_J), \quad (11)$$

where the item Δ 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 [3-5,11,12] is used. All calculations are performed on the basis of the modified numerical code Superatom (version 93).

Results and conclusions

Below we present the advanced data for Au-

ger electron energy in some solids. As mentioned above, the exit probability of Auger electrons from an atom via different channels associated with ionization from a core level is defined by the matrix element (1). In addition, the proportionality coefficient in the equation coincides with the electron impact ionization cross-section σ_j of the level j . Of course, two aspects are to be considered when determining the exit probability of Auger electrons from an atom, namely, the radiative transition under neutralization of a hole at the level j and the possibility of a considerable change in the initial hole distribution at the core levels at the Auger decay via the radiative channel jkl associated as a rule with a considerable distinctions in the non-radiative transition probabilities [11,12]. For definiteness sake, let the ionization of L levels in a multi-electron atom be considered. The probability of the Auger electron emission from the atom via the channel L_3KL (taken as an example) is defined by the ionization cross-section of the level L_3 as well as by a certain effective cross-section depending on the ionization cross-sections of the levels L_p, L_2 . The Auger line intensity is defined by three atomic constants: $A_{jkl} = \sigma_j f_j a_{jkl}$ where a_{jkl} is the non-radiative transition probability; f_j is the Korster-Kronig coefficient; σ_j , the ionization cross-section defined by the matrix element (1) calculated for wave functions of bound state and continuum one. In table 1 we present the data on Auger electron energy for some solids calculated using the presented approach (column C), the semi-empirical method with using the Larkins' equivalent core approximation [8] (column A), the perturbation theory approach [11,12] as well as experimental data (c.g.[1]).

Table 1

Experimental data for Auger electron energy for solids and calculated values (A, semi-empirical method [1]; B, [11,12]; C- present)

Element	Auger line	Experiment	Theory: A	Theory: B	Theory: C
Na	$KL_{2,3}L_{2,3}^1D_2$	994.2	993.3	994.7	994.1
Si	$KL_{2,3}L_{2,3}^1D_2$	1616.4	1614.0	1615.9	1616.2
Ge	$L_3M_{4,5}M_{4,5}^1G_4$	1146.2	1147.2	1146.6	1146.1
Ag	$M_3N_{4,5}N_{4,5}^1G_4$	353.4	358.8	354.1	353.2

The calculation accuracy using method [1] is within about 2 eV as an average. Our approach provides more accurate results that is provided by more correct accounting for complex electron interaction. Some improvement of the present data in comparison with results [9,10] is connected using the optimized one-quasiparticle representation in the relativistic many-body perturbation theory, which significantly affects an agreement between theory and experiment.

To conclude, let us note [12] that using the Auger electron spectroscopy in analysis of the surface chemical composition and elements [1,3,30-34] requires consideration of Auger spectra and the corresponding characteristics of the Auger transitions, interpretation of effects like the shape transformations of the valence Auger spectra due to appearance of new lines, position and intensity changes of individual lines caused by the redistribution in the electron state density of the valence band. The correct theoretical estimations of the spectral characteristics are of critical importance for their full understanding.

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Summary

The Auger electron spectroscopy is an effective method to study the chemical composition of solid surfaces and near-surface layers. Sensing the Auger spectra in atomic systems and solids gives the important data for the whole number of scientific and technological applications. When considering the method principles, the main attention is given as a rule to the models for drawing chemical information from the Auger spectra and to the surface composition determination methods by the Auger spectrum decoding. It is just the two-step model that is used most widely when calculating the Auger decay characteristics. 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 this paper the combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order density functional approximation is applied to determination of the energy and spectral parameters of the Auger decay for the Na, Si, Ge, Ag solids. The results are compared with reported experimental results as well as with those obtained by alternative theoretical schemes. The important point is linked with an accurate accounting for the complex exchange-correlation (polarization) effect contributions and using the optimized one-quasiparticle representation in the relativistic many-body perturbation theory zeroth approximation, which significantly affects the agreement of theory and experiment.

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ТЕОРЕТИЧНА ОЖЕ-СПЕКТРОСКОПІЯ ТВЕРДОГО ТІЛА: РОЗРАХУНОК ЕНЕРГЕТИЧНИХ ПАРАМЕТРІВ

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Реферат

Електронна Оже-спектроскопія є ефективним методом вивчення хімічного складу твердих поверхонь і приповерхневих шарів. Вивчення спектрів Оже в атомних, молекулярних системах і твердих тілах дає важливі дані для багаточисленних науково-технічних застосувань. Як правило,

головна увага приділяється моделям обчислення Оже-спектрів та отриманню інформації про основні енергетичні та спектральні параметри, а також визначенню складу поверхні на основі розшифровки Оже-спектрів. В даній роботі комбінований релятивістський енергетичний підхід і релятивістська багаточастинкова теорія збурень з нульовим наближенням функціонала густини застосовуються для визначення енергетичних і спектральних параметрів Оже-процесу в твердотільних Na, Si, Ge, Ag. Результати порівнюються з узагальненими експериментальними результатами, а також з результатами, отриманими на основі альтернативних теоретичних методів. Важливий момент пов'язаний з коректним урахуванням внесків складних багаточастинкових обмінно-кореляційних ефектів та використанням оптимізованого одночастинкового уявлення в нульовому наближенні релятивістської багаточастинкової теорії збурень, що суттєво впливає на згоду теорії та експерименту.

Ключові слова: релятивістська теорія, Оже-спектроскопія, тверде тіло