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Auger effect in atoms and solids: Calculation of Auger decay characteristics in atoms, quasi-molecules, and solids for the surface composition analysis

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Paper is devoted to calculation of characteristics of the Auger decay in the complicated atomic systems and solids on the basis of S-matrix Gell-Mann and Low formalism. The cross-sections of ionization of the internal shells for a number of atoms (Na, Si, Au) and energies of Auger electron transitions in solids (Na, Si, Ge, Ag) are calculated with account of the correlation effects. Within a non-relativistic approximation of effective potential with using the screened continuum functions it is carried out a calculation of the Auger transition probabilities from a number of states for HeH^+ system. Data obtained are useful for using the Auger electron spectroscopy method for analysis of chemical constitution of the surface.

Работа посвящена расчету характеристик Оже распада в сложных атомных системах, твердых телах на основе метода, базирующегося на S-матричном формализме Гелл-Мана и Лоу. Выполнены расчеты сечений ионизации внутренних оболочек ряда атомов (Na, Si, Au) и энергий Оже электронов в твердых телах (Na, Si, Ge, Ag). В нерелятивистском приближении эффективного потенциала с применением экранированных функций континуума выполнен расчет вероятностей Оже переходов из ряда состояний HeH^+. Полученные данные полезны при использовании метода Оже электронной спектроскопии для анализа химического состава поверхности, связанного с анализом Оже спектров.

The Auger electron spectroscopy is an effective method to study the chemical composition of solid surfaces and near-surface layers [1–5]. 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 [2, 3], 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 redistribution 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. [2–18]. Note that the effects are not described adequately to date, in particular, within the Auger decay theory [6].

In this work, a novel calculation method of Auger decay characteristics for complex atomic systems basing on the S-matrix formalism by Hell-Mann and Law [7–13] is applied to calculation of those characteristics for atoms, molecules, and solids. The novel