

AUGER EFFECT IN ATOMS, SOLIDS AND POSSIBLE APPLICATIONS TO THE CHEMICAL COMPOSITION OF SOLID SURFACES

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The Auger electron spectroscopy is an effective method to study the chemical composition of solid surfaces and near-surface layers [1,2]. Under considering the method principles, it is just the two-step model that is used most widely when calculating the Auger decay (AD) 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 the processes are not believed to be independent from one another. In this paper a novel calculation approach to description of AD characteristics for complex atomic systems basing on the S-matrix formalism [2] is applied to studying characteristics for atoms and solids. The method has been applied to calculate the ionization cross-sections of inner shells in various atoms and the Auger electron energy in solids (*Na, Si, Ge, Ag*). Two aspects are 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 AD via the radiative channel *jkl* associated as a rule with a considerable distinctions in the non-radiative transition probabilities. 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 *L₃Kl* (taken as an example) is defined by the ionization cross-section of the level *L₃* as well as by a certain effective cross-section depending on the ionization cross-sections of the levels *L₁, L₂*. The Auger line intensity is defined by three atomic constants: $A_{jkl} = \sigma_j f_i a_{jkl}$, where a_{jkl} is the non-radiative transition probability; f_i is the Korster-Kronig coefficient; σ_j , the ionization cross-section defined by the matrix element calculated for wave functions of bound state and continuum one. Table presents data on the Auger electron energy for some solids calculated using the method of this paper and the semi-empirical method under Larkins' equivalent core approximation [1] as well as experimental data. Our approach provides more accurate results that is due to a considerable extent to more correct accounting for complex electron interaction. To conclude, note that the use of the Auger electron spectroscopy in analysis of the surface chemical composition requires consideration of Auger spectra, interpretation of effects like the shape transformations of valence Auger spectra due to appearance of new lines and intensity changes of lines caused by redistribution in electron state density of valence band.

Elementr	Auger line	Experiment	Theory [1]	Present
<i>Na</i>	<i>KL_{2,3}L_{2,3}¹D₂</i>	994,2	993,3	994,1
<i>Si</i>	<i>KL_{2,3}L_{2,3}¹D₂</i>	1616,4	1614,0	1615,9
<i>Ge</i>	<i>L₃M_{4,5}M_{4,5}¹G₄</i>	1146,2	1147,2	1146,6
<i>Ag</i>	<i>M₅N_{4,5}N_{4,5}¹G₄</i>	353,4	358,8	354,1

References

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 [2]. A.Glushkov etal, Int.J.Quant.Chem. 99 (2004) 889; 99 (2004) 936; 104 (2005) 562;