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COMPUTER MODELLING OPTIMAL SCHEMES OF THE LASER PHOTOIONIZATION METHOD FOR PREPARING THE FILMS OF PURE COMPOSITION AT ATOMIC LEVEL

The optimal laser photoionization scheme for preparing the films of pure composition on example of creation of the hetero structures (layers of GaAlAs) is proposed.. New model of optimal realization of the first step excitation and further ionization of the As^+ ions in Rydberg states by DC electric field is developed.

Carrying out the effective methods for obtaining especially pure substances or their control and cleaning from admixtures (c.f. [1,2]) is considered as one of the actual problem of modern technology of the semiconductor and other materials. In particular, speech is about methods for control of the Al, B admixtures in Ge and other third group acceptor elements admixtures at the level of 10^{-8}–10^{-10}%. In some cases the similar sensitivity may be provided by traditional analytic methods [1] or their modifications. However, its sensitivity is limited by level of 10^{-7}%. Selective photo physics methods (c.f. [2–17]) allow to develop a new approach to technologies of obtaining the pure substances at atomic level and solving many other problems. The basis for its successful realization is, first of all, in carrying out the optimal multi stepped photoionization schemes for different elements and, at second, availability of enough effective UV and visible range lasers with high average power. Our paper is devoted to the search and computer modeling the optimal schemes of laser photoionization method for control and cleaning the semiconducting substances. We will carry out modeling the laser photoionization scheme for preparing the films of pure composition on example of creation of the hetero structural super lattices (layers of $Ga_{1-x}Al_xAs$ with width 10E and GaAs of 60E). New models of optimal realization of the first step excitation and further ionization of the As^+ ions in Rydberg states by electric field are proposed and optimal parameters of the photo ionization process are found. Similar studying for Al and Ga ions had been carried out earlier [8–10].

The possible scheme for preparing the films of pure composition by means of the two-stepped selective ionization of atoms has been proposed by V. Letokhov [2]. Such scheme was not experimentally checked, however it is obvious that the two-stepped laser ionization scheme is not optimal one (see explanation below). The main innovation of our scheme is connected with using the electric field ionization pulse on the last ionization step. In ref. [8–10] we carried out modelling the optimal scheme for laser photoionization scheme of control and cleaning the substance and preparing pure films on atomic level for a number of elements, including Ga, Al etc. In a classic scheme, the laser excitation of admixture atoms is realized at several steps: atoms are resonantly excited by laser radiation and then it is realized photo ionization of excited atoms (c.f. [2-8]). In this case photo ionization process is characterized by relatively low cross section $\sigma_{ion}=10^{-17}$–$10^{-18}cm^2$ and one could use the powerful laser radiation on the ionization step. Alternative mechanism is a transition of atoms into Rydberg states and further ionization by electric field. As result, the requirements to energetics of ionized pulse are decreased at several orders.

As usually, the elements separation process is described by corresponding master system of equations for density matrice [2,8]. We supposed that a laser radiation acts on the admixtures atom and concentration of admixtures is quite little. The resonant exchange probability is less than ionization velocity, i.e. $W_2 > \sigma_w$ vN (N- concentration of atoms) and the ions yield time from neutral atom cloud is less than re-charging time, i.e.: $N\sigma_{ch}d<1$. At first step, the photo-ionization scheme includes an excitation of atoms by laser field and their transition into Rydberg states and then ionization by electric field. A creation of the films of pure composition (creation of the 3-D layers of $Ga_{1-x}Al_xAs$ with width 10E and GaAs of 60E) is directly connected with using the photo ion pensils of Ga^+, Al^+, As^+. Similar pensils can be created by means of the selective photoionization method with ionization by electric field. Then electromagnetic focusing and deflecting systems will provide creation of the 3-D supper lattices (c.f.[2]).

We consider the ionization scheme of obtaining the As^+ ions. The transition scheme is as follows; $4p^3\ {}^4S_{3/2} \rightarrow (50693{,}9cm^{-1}) \rightarrow 5s^4P_{1/2} \rightarrow (\lambda_2[n]) \rightarrow np^{32}D_{3/2}$ (n=10-25). We carried out modeling the optimal parameters for last process, i.e. ionization of the Rydberg states by electric field. In figure 1 we present results of modeling the As atoms separation process by solving system (1). All necessary constants are preliminarily calculated and taken from refs [2, 3, 8–10, 15–17]. The following definitions are used: δ+dashed line is corresponding to optimal form of laser pulse, curves 1 and 2 are corresponding to populations of the ground and excited states of As. The δ -pulse provides maximum possible level of excitation (the excitation degree is about ~0,2; in experiment [2] with rectangular pulse this degree was ~ 0,1. In further the parasite processes

such as spontaneous relaxation, resonant re- exchange can't change the achieved excitation level during a little time. The last step of the process is an ionization of excited atoms by the electric field pulse.

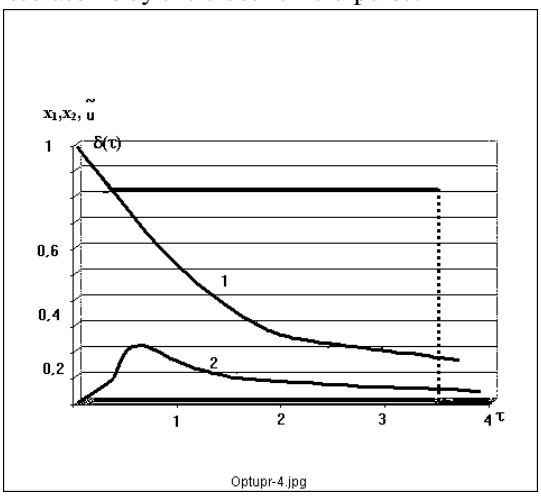

Fig. 1 Results of modeling As separation process by photoionization method (δ+dashed – laser pulse optimal form; curves 1, 2 are corresponding to populations of the ground and excited states)

It is natural that in order to get a high level of the optimality an electric field has to be switched on during the time, which is less than the excited state radiative decay time. In figure 2 we present the results of our calculating dependence of the ionization velocity for high excited atoms of As upon the electric field strength for states with quantum numbers n= 10–16. The dashed line is corresponding to velocity of the radiative decay.

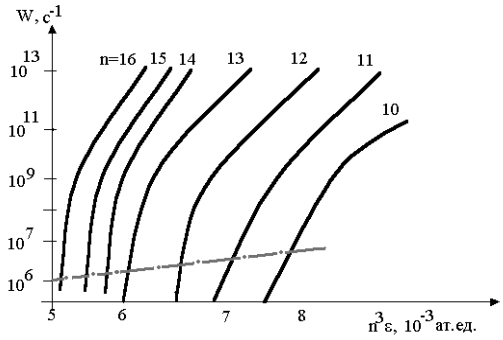

Fig. 2. Dependence of the velocity of ionization for high excited atoms of As on an electric field strength for states with quantum numbers n=10–16

The decay of As atoms and ions in the high-excited state demonstrates qualitatively the properties of the H-like systems. However, there is quite significant quantitative difference. Indeed, the same situation takes a place for Al, Ga elements etc (c.f. [8]). Our estimate for the As atom ionization cross section is $1{,}2\cdot10^{-13}$cm^2 that is higher than the corresponding cross section of ionization process by laser pulse in the two- stepped scheme ($\sim10^{-17}$cm^2 [2]). Using δ-pulse provides a quick ionization, but the ionization yield will be less than 100% because of the sticking on intermediate levels. Experimentally obtained dependence of the critical ionization field strength E upon the effective quantum number n* is usually approximated by simple theoretical dependence $E_{cr}=(2n^*)^{-4}$. However, our calculation results show that this is not very exact approximation and only sophisticated quantum calculation [8–10] provide excellent agreement with experimental data. In any case, the laser photoionization scheme with ionization by electric field could provide significantly more high yield and effectiveness of the whole process than the other known schemes [2]. Naturally, the optimal set of energetic and radiative parameters (pulse form, duration, energetic for laser and electric field pulses etc) should be used. The scheme can be applied in the laser photo ionization technologies for preparing the pure composition films, pure hetero structural super lattices, selective creating photo ions of B, As, P and other elements in equipment for ion legating the semiconductors. It is obvious that the optimal governing approaches may be also useful in a search of optimal realization of the photo-excitation and ionization processes in a number of tasks in molecular, semiconductors, surface physics etc.

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КОМП'ЮТЕРНЕ МОДЕЛЮВАННЯ ОПТИМАЛЬНИХ СХЕМ ЛАЗЕРНОГО ФОТОІОНІЗАЦІЙНОГО МЕТОДУ ДЛЯ ПРИГОТУВАННЯ ПЛІВОК ЧИСТОГО СКЛАДУ НА АТОМНОМУ РІВНІ

Запропоновано оптимальну лазерно-фотоіонізаційну схему приготування плівок особливо чистого складу на прикладі контролю побудови гетероструктур (типу GaAlAs).Розвинуто нову модель оптимальної реалізації збудження на 1-й стадії й подальшої іонізації іонів As^+ у рідбергових станах електричним полем

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КОМПЬЮТЕРНОЕ МОДЕЛИРОВАНИЕ ОПТИМАЛЬНЫХ СХЕМ ЛАЗЕРНО-ФОТОИОНИЗАЦИОННОГО МЕТОДА ПРИГОТОВЛЕНИЯ ПЛЕНОК ОСОБО ЧИСТОГО СОСТАВА НА АТОМНОМ УРОВНЕ

Предложена новая оптимальная лазерно-фотоионизационная схема приготовления пленок особо чистого состава на атомном уровне на примере контроля приготовления гетероструктур (типа GaAlAs). Развита новая модель оптимальной реализации возбуждения на первой стадии и дальнейшей ионизации ионов As^+ в ридберговых состояниях внешним электрическим полем.