ПРОЕКТУВАННЯ І МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ СЕНСОРІВ

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SENSING A DYNAMICS OF THE LASER FIELD ROTATIONAL EXCITATION FOR MOLECULES AND POSSIBLE USING IN LASER PHOTOIONIZATION CLEANING SEMICONDUCTOR SURFACES

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Abstract

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Within the optimal governing theory a problem of sensing rotational excitation, photo ionization and dissociation for molecules in a laser field is studied. A new multi-level optimized model for definition of the optimal form of laser pulse to reach the maximal effectiveness of laser action in process of selective molecule excitation and ionization is used in calculation the parameters of the optimal excitation for molecule *HBr.* The dependence (number of particles) of functional of the quality on the rotational energy and wave length of laser radiation is calculated.

Key words: sensing rotational excitation, molecules in a laser field.

Резюме

ДЕТЕКТУВАННЯ ДИНАМІКИ РОТАЦІЙНОГО ЗБУДЖЕННЯ МОЛЕКУЛ У ПОЛІ ЛАЗЕРНОГО ВИПРОМІНЮВАННЯ ТА МОЖЛИВЕ ВИКОРИСТАННЯ У ЛАЗЕРНО-ФОТОІОНІЗАЦІЙНОМУ МЕТОДІ ОЧИЩЕННЯ НАВІВПРОВІДНИКОВИХ МАТЕРІАЛІВ

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Розглянуто проблему детектування динаміки ротаційного збудження, іонізації та дисоціації молекул у полі лазерного випромінювання у межах теорії оптимального керування. Нова багаторівнева оптимізаційна модель визначення оптимальної форми лазерного імпульсу для досягнення максимальної ефективності лазерної дії у процесі селективного збудження та іонізації молекул використана у розрахунку параметрів оптимального збудження молекул *HBr.* Розраховано залежність функціоналу якості (число частинок) від величини ротаційної енергії та довжини хвилі лазерного випромінювання.

Ключові слова: детектування ротаційного збудження, молекули у лазерному полі

Резюме

ДЕТЕКТИРОВАНИЕ ДИНАМИКИ ВРАЩАТЕЛЬНОГО ВОЗБУЖДЕНИЯ МОЛЕКУЛ В ПОЛЕ ЛАЗЕРНОГО ИЗЛУЧЕНИЯ И ВОЗМОЖНОЕ ИСПОЛЬЗОВАНИЕ В ЛАЗЕРНО-ФОТОИОНИЗАЦИОННОМ МЕТОДЕ ОЧИСТКИ ПОЛУПРОВОДНИКОВЫХ МАТЕРИАЛОВ

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Рассмотрена проблема детектировнаия динамики вращательного возбуждения, ионизации и диссоциаиий молекул в поле лазерного излуения в рамках теории оптимального управления. Новая многоуровневая оптимизационная модель определения оптимальной формы лазерного импульса для достижения максимальной эффективности лазерного воздействия в процессе селективного возбуждения и ионизации молекул использована в расчете параметров оптимального вращательного возбуждения молекул *HBr*. Рассчитана зависимость функционала качества (число частиц) от величины вращательной энергии и длины волны лазерного излучения.

Ключевые слова: детектирование вращательного возбуждения, молекулы в поле лазерного излучения.

Introduction

A significant progress in the development of laser technique stimulated a great interest to carrying out new non-linear optical, laser devices for solving a wide number of tasks in different applications (atomic, molecular chemical physics, quantum electronics, physics of elements, devices, sensor technologies, etc.). Above cited problems is of a great importance in studying of dynamics of the multi-atomic molecules in a strong laser field. A variety of multi-photon processes have been observed in molecules, including multi-photon excitation, ionization, dissociation (c.f.[1-15]). It is very important to note that using lasers allows highly selective introducing the energy quantities into definite freedom degrees of system. It can be used as physical basis for creation and construction of special devices for sensing physical, chemical properties of the molecular systems and can find application in solving problems of the nano-electronics, nano-atomic optics, quantum computing, molecular sensors technologies etc.

Search of the optimal conditions of excitation and ionization for atoms and molecules in laser field attracts a great interest [1-12]. It is well known that a method of selective photo ionization and dissociation of molecules is one of the most effective approaches to solving problem of the laser separation of isotopes and cleaning the semiconductor materials from molecular admixtures. In particular, in Los Alamos laboratory it was at first demonstrated a possibility of selective one-quantum dissociation of admixture molecules (PH_4 and others) by UV radiation of *ArF* excimer laser under action on molecules SiH_4 (c.f.[2]). Laser cleaning of the mono-silan represents a great practical interest for technology of obtaining poor *Si* in the semiconductor industry. A possibility of cleaning the substance in a gas phase by means of the photodissociation of admixtured molecules in IR laser field has been experimentally demonstrated by Letokhov et al [2,3] on the example of cleaning $AsCl_3$ from admixtures $C_2H_4Cl_2$ and CCl_4. Perspective of using the optimal IR-UV photoionization and photo dissociation schemes attracts a great interest. Now a great attention is attracted to theoretical and experimental studying of optimal realizations of processes of the multi-step and multi photon excitation and ionization, dissociation. Though many of cited processes are quite satisfactorily described (at least, at qualitative level) by simplified models. A majority of tasks for action of laser radiation and high intensive particles beams on molecular gases are quite acceptably described by multi- level models, which result in systems of differential equations or differential equation in partial derivatives of the Focker-Plank type [3,7,8,14]. But, a consistent theory of the optimal realizations of these processes is absent. In refs. [13-15] within the optimal governing theory a problem of optimization for electron, vibtational and rotational excitation, photoionization and dissociation in a laser field has been studied and a new multi-level optimized model for definition of the optimal form of laser pulse to reach the maximal effectiveness of laser action in process of selective

excitation and ionization of molecules has been proposed. As example, the parameters of the optimal excitation and ionization for molecules *HCl,* CF_3Br(I), SiH_4 *etc.* have been determined. Here we present the results of analogous calculation for *HBr* molecule, namely, it is calculated a dependence (number of particles) of functional of the quality on the rotational energy and wave length of laser radiation. Let us also note that an approach considered can be used in tasks of choosing the optimal parameters of the selective photoionization method for cleaning the semiconductor materials from surface molecule admixtures [14,15].

Optimal model of rotational excitation of molecules

At once let us formulate the basic moments of our model, following to refs.[14,15]. Numerical procedure is based on the finite differences scheme FDS-2 (see details in [14,20]). The model is based on differential equation of the Focker-Plank type:

$$\partial f / \partial t = L_{RT} + L_u(f, I) \tag{1}$$

where f is a density of molecules at a chosen vibration level with rotational energy x; I is a laser pulse intensity; $L_{RT}, L_u(f,I)$ are operators, which describe the RT relaxation and laser radiation action:

$$L_{RT}(f) = \partial^2 f/\partial x^2 + \partial f/\partial x, ..., L_u = \\ = I(x,t)u(t)(f(x_2,t) - f(x_1,t)) \tag{2}$$

At initial moment of time there is some initial distribution $f(x,0)$, and for t>0 system is excited by resonance laser field with frequency, which is resonant to rotational transition $x_1 \to x_2$. We consider a frequency of the exciting field as governing parameter. To estimate an effectiveness of action one must study a quality functional, which characterises a distribution of molecules on rotational energies to moment t_1:

$$Y(u) = \int_0^R f(x, t_1; u) h(x) dx \tag{3}$$

where $h(x)$ is some function, which corresponds to required form of the final distribution. Further we are dealing with real form of the laser pulse. As the experiments on studying laser action on substance have shown, an adequate approximation for description of laser pulse form has the following form see [2,3]):

$$I(t) \sim \begin{pmatrix} \Phi_1/\tau_1, \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 0 < t < \tau_1, \\ (2\Phi_2/\tau_2)\{1 - [(t-\tau_1)/\tau_2]\}^2, \ldots\ldots \tau_1 < t < \tau_1 + \tau_2 < t_1 \end{pmatrix} \tag{4}$$

where Φ_1 and Φ_2 are the values of the laser pulse power, τ_1 and τ_2 are some times (the values of these parameters are taken from experiment). In a principle, a search for the optimal form of the laser pulse is separated problem. The optimal governing task for definition of the optimal laser pulse form to achieve a maximal laser action effectiveness is written as follows [15]:

$$\begin{gathered} \partial f / \partial t = \partial^2 f/\partial x^2 + \partial f/\partial x + \\ + I(x,t)u(t)(f(x_2,t) - f(x_1,t)) \\ f(x,0) = f_0(x), \ldots\ldots\ldots\ldots 0 < x < R, \\ \partial f/\partial x + + f|_{x=0,R} = 0, \ldots . 0 < t < t_1 \end{gathered} \tag{5}$$

With using conjunction task one could write a necessary condition of optimality: if (x_1^*, x_2^*) is an optimal governing for functional (3) and $f^*(x,t), \Psi^*(x,t)$ are corresponding solutions, then we have the following condition for any x_1, x_2 from interval [0,R]:

$$Y'_{x_1}(x_1^*, x_2^*, f^*, \Psi^*)(x_1 - x_1^*) + \\ + Y'_{x_2}(x_1^*, x_2^*, f^*, \Psi^*)(x_2 - x_2^*) \le 0$$

Numerical results and conclusions

We have carried out the numerical testing of the model (1-5) for molecules *HBr* (T=300 K, R=25; the values of parameters are taken from refs.[2-4,7]). In figure 1 a dependence (number of particles) of the functional is presented:

$$I(u) = \int_0^R f(x, t_1; x_1, x_2) h(x) dx \tag{6}$$

in the interval of energies $x \in [13,25]$ (in units of kT) upon x_1 and wavelength of laser radiation, which is corresponding to rotation transition $x_1 \to x_2$. In expression (4) h is a function, which corresponds to required form of the final distribution f(x,t,u), i.e. density of molecules at chosen vibration level, which

has a rotational energy x at moment of time t; $x \in [0, R]$). It is found the optimal set of physical parameters to provide an optimality of process, in particular, at wave length λ=0,16μm it has taken place the optimal regime of excitation process. The obtained data are qualitatively similar to results of ref. [14,15]for molecule *HCl, CF_3Br*. The quantitative difference is provided by using the real laser pulse form (3) and molecular constants set. The similar calculation is now in progress for molecule PH_3 under the UV laser field action on silane surface. It is obvious that using of optimized models of excitation, ionization and photodissociation of molecules may improve general technologies of laser cleaning the semiconductors materials from admixtures and substances in a gas phase by means of method of photo dissociation of the admixture molecules in a laser field.

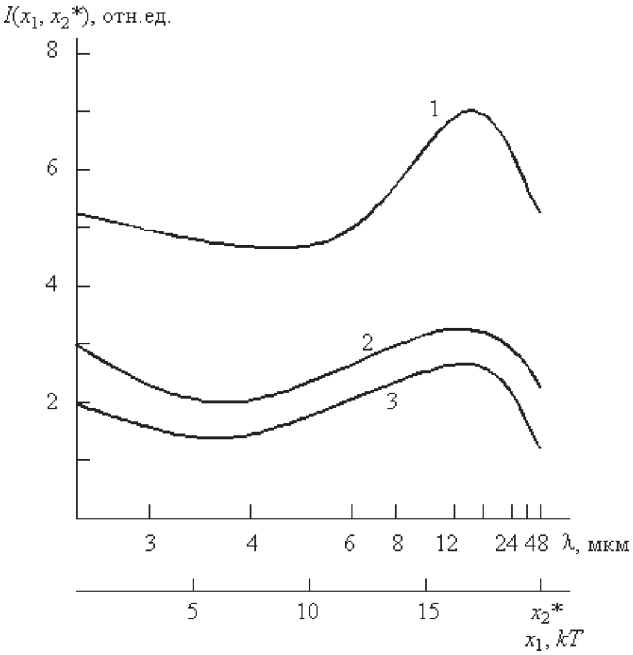

Fig.1. Dependence of the functional $I(x_1, x_2)$ upon x_1 and wave length of laser radiation for $t_1=2\tau_R$ (1), $t_1=4\tau_R$ (2), $t_1=6\tau_R$ (3) for molecule *HBr* (see text)

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