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Selective photoionization and photodissociation of molecules for purification of semiconductor materials and substances in gas state: optimized scheme

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The optimization problems of rotational excitement, photoionization and photodissociation under laser irradiation are considered basing on the optimum control theory. A new multi-level optimized model is presented for determination of the optimum laser pulse shape to provide the maximal efficiency of laser action in the selective photoionization (photodissociation) of molecules based on Focker-Plank type differential equation and optimum control theory method. As an example, the conditions and parameters for optimum excitement and photodissociation are determined for HCl and CF_3Br molecules. The dependence of the quality functional (number of particles) on the sought-for energy and laser radiation wavelength is calculated within an interval of rotational energy values (in kT units). The approach elaborated forms a base for choosing the optimum parameters of the selective photoionization and photodissociation of molecules for semiconductor materials purification from molecular impurities.

На основе теории оптимального управления рассмотрен класс задач оптимизации вращательного возбуждения, фотоионизации, фотодиссоциации молекул под действием лазерного излучения. Предложена новая многоуровневая модель определения оптимальной формы лазерного импульса для достижения максимальной эффективности процесса селективной фотоионизации (фотодиссоциации) молекул, базирующаяся на использовании уравнения типа Фоккера-Планка и теории оптимального управления. В качестве примера определены условия и параметры оптимального возбуждения и фотодиссоциации для молекул HCl и CF_3Br, в частности, рассчитана зависимость функционала качества в задаче оптимального управления (числа частиц) в интервале вращательных энергий (в единицах kT) от величины искомой энергии и длины волны лазерного излучения. Развитый подход лежит в основе выбора оптимальных параметров метода селективной фотоионизации и фотодиссоциации молекул для очистки полупроводниковых материалов и веществ в газовой фазе от примесей.

One of the most effective approaches to the solution of laser separation for isotopes and nuclear isomers is provided by selective ionization of atoms and molecules based on the selective resonance excitation of atoms by laser radiation into states near the ionization threshold and further photoionization of the excited states by additional laser radiation field or ionization of the autoionizing resonances by an electric field [1–6]. The method was at first proposed and realized in laboratory conditions by Letokhov [4]. Selective photoionization and photodissociation of molecules is supposed to be a method of very good prospects for purification of semiconductor materials from molecular admixtures. In particular, in Los Alamos Laboratory, a possibility of selective one-quantum dissociation was demonstrated at first for impurity molecules (PH_4 and other) by UV radiation of ArF excimer laser affecting SiH_4 molecules [7]. Laser purification of mono-silan is of a great practical interest for pure Si production in the semiconductor industry.