

сред, при хорошей емкостной связи антенны со средой. В случае измерений в сухих почвах возможно возникновение паразитных колебаний.

На основе полученных результатов экспериментов, проведенного анализа и дополнительных измерений была разработана антенна, приведенная на рис.2 под №9. Для длины 50 см и ширины 3,4 см применена плавная трапеция, длина сегментов уменьшается по экспоненте, количество сегментов равно пяти, в качестве резисторов используются чип-резисторы размера 1206. Применено параллельное включение 4 резисторов, при импульсной амплитуде передатчика 5 кВ и длительности до 15 нс они надежно работают. Диаграмма направленности антенны приблизительно равна характеристикам антенны №6 и здесь не приводится. Эксперименты показали, что для решения конкретно поставленных задач можно путем изменения геометрических параметров антенн находить их наиболее оптимальные варианты конструкций с наилучшими радиотехническими характеристиками.

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CALCULATING THE VALUES OF THE DIPOLE MOMENTS OF ELECTRONIC TRANSITIONS

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ANNOTATION

In this work, the values of dipole moments of electron transitions are calculated using the semiempirical method, taking into account the rotation of the molecule analytically (through $3j$ - and $6j$ -semivolts). Integrals of the intersection of vibrational wave functions of combining States are found. The absolute values of dipole moments of electronic transitions $3l^3 A'_g \rightarrow 2p^3 A''_u$ necessary for calculating the coefficients of expansion of the wave function of the perturbed state of a triplet $3s, 3d$ - complex of terms on the born-Oppenheimer basis and the overlap integrals of the number of negative wave functions corresponding to radiation transitions are determined. Using χ^2 the difference standard calculated by formulas optimization subroutine FUMIL the effective values of dipole moments of electronic components were determined $3l^3 A'_g \rightarrow 2p^3 A''_u H_2$.

Keyword: dipole moments electron transitions, wave function, overlap integrals, electronic levels.

The task of this paper is to find the values of dipole parameters by a semiempirical method.

To solve this problem, the rotation of the molecule was taken into account analytically (through $3j$ - and $6j$ -semivolts), and the critical integrals of vibrational wave functions of combining States were determined numerically.

Research of relative values of probabilities of electron-vibrational-rotational (EQ) transitions from the levels of the triplet $3s, 3d$ -complex of terms of the

hydrogen molecule were performed semi-empirically [1].

Using laser-stimulated photo fragmentation spectroscopy, we found the probability ratios of spontaneous transitions from the EQ levels $3l^3 A'_g$ - from the preassociating $b^3 \Sigma_u^+$ - state $c^3 \Pi_r^+$ - positions and the orbital quantum numbers of the valence electron in the corresponding unified atom Λ - a literal designation of the quantum number of the electron momentum projection operator on the inter-core axis. This method is based on the registration of the speed

spectrum of atoms formed during spontaneous transitions to unstable States[2-4]. Non-adiabatic calculations, which used nonempirical dependences of the total moments of electronic transitions $3l^3A'_g \rightarrow 2l^3A''_u$, led to a discrepancy with experimental values [5-6].

The semi-empirical analysis of these data made it possible to find the relative adiabatic values of the dipole moments of these electronic transitions. In addition, the results of our semi-empirical analysis of the force relations of the lines of various rotational branches of the electron-vibrational transition bands $j^3A'_g \rightarrow c^3\Pi_u^\pm$ were in good agreement with the values measured by laser-induced fluorescence [7]. When describing the probabilities of transitions from the levels of the triplet $3s, 3d$ -complex of terms of the hydrogen molecule, we will adhere to the formalism, developed by us when analyzing the relative probabilities of spontaneous transitions [8].

The formulas are based on the account of EQ level interactions only with the same values of vibrational and rotational quantum numbers in a closed triplet $3s, 3d$ -complex of terms. In this case, the spin multiplet splitting of the levels is considered to be much smaller than the value of the effects associated with electron-vibrational and electron-rotational interactions. We will neglect the interaction $b^3\Sigma_u^+$, of both $c^3\Pi_u^+$ – the States at which radiation transitions occur, and the dependences of the dipole moments $3l^3A'_g \rightarrow 2p^3A''_u$ of

electronic transitions on the inter-nuclear distance. Taking these assumptions into account the formula for the probability of a spontaneous transition $\gamma, v', N' \rightarrow c^3\Pi_u, v'', N''$. Previously, we used a semi-empirical method to study the force relations of the lines of R -, Q -, and P -branches $3l^3A'_g, v, N' \rightarrow c^3\Pi_u^\pm, v, N''$ – transitions and determined the values of three relations of dipole moments of electron beams:

$$3s^3\Sigma_g \rightarrow 2p^3\Pi_u, \quad 3d^3\Sigma_g \rightarrow$$

$$2p^3\Pi_u, \quad 3d^3A_g \rightarrow 2p^3\Pi_u \text{ to}$$

the dipole moment of transition $3d^3\Pi_g \rightarrow 2p^3\Pi_u$ –

$$M_{2p\Pi}^{3s\Sigma} / M_{2p\Pi}^{3d\Pi} = 0.28 \pm 0.01,$$

$$M_{2p\Pi}^{3d\Sigma} / M_{2p\Pi}^{3d\Pi} = -0.82 \pm 0.02,$$

$M_{2p\Pi}^{3d\Pi} / M_{2p\Pi}^{3d\Pi} = -1.37 \pm 0.02$. These values are used to describe the lifetime of electron-vibrational-rotational (EQ) have a smooth triplet $3s, 3d$ -complex the MOU. The expression for the radiative lifetimes of the γ, v', N' . The EQ of the levels of the triplet $3s, 3d$ -complex of terms caused by spontaneous transitions to electronic States resolved in the dipole approximation $b^3\Sigma_u^+, c^3\Pi_u^\pm, e^3\Sigma_u^+$ and $d^3\Pi_u^\pm$, has the following form:

$$\tau_{\gamma v' N'}^{rad} = \left\{ A_b^{\gamma v' N'} + \sum_{v'', N''} \left(A_{cv'' N''}^{\gamma v' N'} + A_{ev'' N''}^{\gamma v' N'} + A_{dv'' N''}^{\gamma v' N'} \right) \right\}^{-1}, \quad (1)$$

where γ denotes the set of quantum numbers that characterize the electron state; $A_b^{\gamma v' N'}$, $A_{cv'' N''}^{\gamma v' N'}$, $A_{ev'' N''}^{\gamma v' N'}$, $A_{dv'' N''}^{\gamma v' N'}$ – the probabilities of spontaneous transitions from $\gamma, v' N' -$, $b^3\Sigma_u^+, c^3\Pi_u^\pm, v'', N'' -$, $e^3\Sigma_u^+, v'', N'' -$ and $d^3\Pi_u^\pm, v'', N'' -$ the state.

For transitions to stable EQ States, the probabilities of transitions along different rotational branches of the electron-vibrational bands of the progression are summed up in formula (1) в ветвях электронно-колебательных полос $v'' -$.

In the case of transitions to the $b^3\Sigma_u^+$ – state, it is necessary to integrate the probability density over the

continuous spectrum of frequency-emission at the transition from this level. Since the wave number, the diagonal bands of transitions $\gamma, v' N' \rightarrow (e^3\Sigma_u^+, d^3\Pi_u^\pm)$, v'', N'' from the levels of the triplet $3s, 3d$ -complex terms to the levels of the triplet $3p$ -complex terms at least 3 times less than the wave number of the transitions in the $b^3\Sigma_u^+$, and $c^3\Pi_u^\pm$ -state, and the probability of radiative transitions is known to have a cubic dependence on the magnitude of the wave number, then the further analysis we will not consider the transitions from these levels $e^3\Sigma_u^+$ and $d^3\Pi_u^\pm$ – condition:

$$\begin{aligned} A_{cv'' N''}^{\gamma v' N'} &= \frac{64\pi^4}{3h} \left(c_{cv'' N''}^{\gamma v' N'} \right)^3 (2N' + 1)(2N'' + 1)^2 \times \\ &\times \left\{ \begin{matrix} N' & 0 & N' \\ N'' & 1 & N'' \end{matrix} \right\}^2 c_{3s\Sigma}(\gamma, v' N') M_{2p\Pi}^{3s\Sigma} \times \\ &\times \langle 2p\Pi, v'' N'' | 3s\Sigma, v' N' \rangle_0 \begin{pmatrix} N' & 1 & N'' \\ 0 & -1 & 1 \end{pmatrix} + \\ &+ c_{3s\Sigma}(\gamma, v' N') M_{2p\Pi}^{3d\Sigma} \times \\ &\times \langle 2p\Pi, v'' N'' | 3d\Sigma, v' N' \rangle_0 \begin{pmatrix} N' & 1 & N'' \\ 0 & -1 & 1 \end{pmatrix} + \\ &+ c_{3d\Pi}(\gamma, v' N') M_{2p\Pi}^{3d\Pi} \times \\ &\times \langle 2p\Pi, v'' N'' | 3d\Sigma, v' N' \rangle_0 \begin{pmatrix} N' & 1 & N'' \\ -1 & 0 & 1 \end{pmatrix} + \end{aligned}$$

$$+c_{3d\Delta}(\gamma, v'N')M_{2p\Pi}^{3d\Delta} \times \langle 2p\Pi, v''N''|3d\Delta, v'N'\rangle_0 \begin{pmatrix} N' & 1 & N'' \\ -2 & 1 & 1 \end{pmatrix}, \quad (2)$$

where

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} + \begin{pmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{pmatrix}$$

$$A_b^{\gamma v'N'} = \frac{64\pi^4}{3h} (2N' + 1) \left(\int_0^\infty v^3 \langle 3L\Lambda, v'N'|b, v\rangle_0 dv \right) \times$$

$$\sum_{N''} (2N'' + 1)^2 \left\{ \begin{matrix} N' & 0 & N'' \\ N'' & 1 & N'' \end{matrix} \right\}^2 \left| c_{3s\Sigma}(\gamma, v'N')M_{2p\Sigma}^{3s\Sigma} \times \right.$$

$$\times \begin{pmatrix} N' & 1 & N'' \\ 0 & 0 & 0 \end{pmatrix} + c_{3d\Sigma}(\gamma, v'N')M_{2p\Sigma}^{3d\Sigma} \begin{pmatrix} N' & 1 & N'' \\ 0 & 0 & 0 \end{pmatrix} +$$

$$\times c_{3d\Pi}(\gamma, v'N')M_{2p\Pi}^{3d\Pi} \begin{pmatrix} N' & 1 & N'' \\ -1 & 1 & 0 \end{pmatrix} \quad (3)$$

where $M_{2p\Sigma}^{3s\Sigma}, M_{2p\Sigma}^{3d\Sigma}$ и $M_{2p\Pi}^{3d\Pi}$ - dipole moments of transitions from $3l^3\Lambda_g$ -States to $2p^3\Sigma_u$, -state, and integration in formula (3) is carried out over the entire region of change in the wave number of the radiation transition of the molecule from $3l^3\Lambda_g, v', N'$ - to the unstable $b^3\Sigma_u^-$ -state [8].

To determine the values of the dipole moments of electronic transitions $3l^3\Lambda_g \rightarrow 2p^3\Lambda_u''$, the coefficients of the expansion of the wave function of the perturbed state of the triplet $3s, 3d$ - complex of terms are required. Therefore we were determined via born-oppingaeroscope basis and the integrals of the overlap of the vibrational wave functions corresponding to the

radiation goon ladies[9]. Knowing the values of the four dipole moments of electronic transitions $3d^3\Pi_g \rightarrow 2p^3\Pi_u, 3s^3\Sigma_g \rightarrow 2p^3\Sigma_u, 3d^3\Sigma_g \rightarrow 2p^3\Sigma_u$, and $3d^3\Pi_g \rightarrow 2p^3\Sigma_u$ $M_{2p\Pi}^{3d\Pi}, M_{2p\Sigma}^{3s\Sigma}, M_{2p\Sigma}^{3d\Sigma}$ и $M_{2p\Sigma}^{3d\Pi}$.

These values were considered as four independent parameters, which, within the framework of the model used, should describe the radiation lifetimes of EQ levels of the triplet $3s, 3d$ -term complex.

Using χ^2 the mean-square differences calculated by the formulas (1) - (3) using the standard optimization subroutine FUMIL были определены FUMIL, the effective values of dipole moments were determined click $3l^3\Lambda_g' \rightarrow 2p^3\Lambda_u''H_2$.

Table 1

Electronic Transition	ζ	Electronic dipole moments of the transitions a. e.						χ_{\min}^2	
		$M_{2p\Sigma}^{3s\Sigma}$	$M_{2p\Sigma}^{3d\Sigma}$	$M_{2p\Sigma}^{3d\Pi}$	$M_{2p\Pi}^{3s\Sigma}$	$M_{2p\Pi}^{3d\Sigma}$	$M_{2p\Pi}^{3d\Pi}$		$M_{2p\Pi}^{3d\Delta}$
$i^3\Pi_g^-, j^3\Delta_g^- \rightarrow c^3\Pi_u$	15	-	-	-0.50(2)	-	-	1.87(3)	-2.56(6)	1.1
$h^3\Sigma_g^+, g^3\Sigma_g^+, i^3\Pi_g^+, j^3\Delta_g^+ \rightarrow c^3\Pi_u$	12	-0.12(1)	0.39(2)	-0.56(4)	0.54(2)	-1.63(3)	1.94(3)	-2.66(6)	6.1
$h^3\Sigma_g^+, g^3\Sigma_g^+, i^3\Pi_g^\pm, j^3\Delta_g^\pm \rightarrow c^3\Pi_u$	27	-0.12(1)	0.40(2)	-0.52(2)	0.54(2)	-1.61(3)	1.92(2)	-2.63(6)	3.5
Range r , a. e.	-	1.6 - 2.7	1.5 - 2.8	1.6 - 2.7	1.6 - 2.7	1.5 - 2.8	1.6 - 2.7	1.5 - 3.0	
Semi-empirical data [9] for $r = 1$ a. e.	21	0.65	-0.50	-0.65 $\sqrt{2}$	0.21 $\sqrt{2}$	0.17 $\sqrt{2}$	1.86	-2.48	
Rating (HeI) [9]	-	1.269	2.170	-1.880 $\sqrt{2}$	1.269 $\sqrt{2}$	-1.085 $\sqrt{2}$	1.880	-2.658	
Rating (HI) [9]	-	0.542	2.452	-2.123 $\sqrt{2}$	0.542 $\sqrt{2}$	-1.226 $\sqrt{2}$	2.123	-3.003	

Thus, the empirical calculations of the values of radiation lifetimes of States using the studied values of dipole moments of electron transitions are in good agreement with the existing experimental data[10].

A comparison of the results obtained separately for $3\Lambda_g^-$ и $3\Lambda_g^+$ - the States of the $3s, 3d$ -complex of terms H_2 shows a good agreement of the values of the dande moments of the electronic transitions $3d^3\Pi_g \rightarrow 2p^3\Sigma_u$ and $3d^3\Pi_g \rightarrow 2p^3\Pi_u$.

Results :

1.The values of the dipole moments of electron transitions are calculated by the semiy-empirical method, taking into account the rotation of the molecule analytically (including $3p\epsilon_3$ $3j$ -and $6j$ -semivoles).

2.Integrals of overlap of oscillatory wave functions of combining States are found.

3. absolute values of dipole moments of electronic transitions are Determined $3l^3\Lambda_g' \rightarrow 2p^3\Lambda_u''$.

4. The effective values of the dipole moments of electronic components are calculated $3l^3 A_g' \rightarrow 2p^3 A_u'' H_2$.

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К ВОПРОСУ ОБ ОБРАТНОМ ЭФФЕКТЕ ХОЛЛА-ПЕТЧА

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TO THE QUESTION ABOUT HALLA-PATCH BACK EFFECT

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АННОТАЦИЯ

До настоящего времени дискутируется эмпирический закон Холла-Петча и его обратный эффект. Предложены многочисленные модели и показана неисчерпаемость глубокой концепции Холла-Петча. В рамках настоящей работы, мы хотим показать, что обратный эффект Холла-Петча наблюдается не только в поликристаллах, но присущ и атомарно-гладким нанокристаллам. Для определения толщины поверхностного слоя атомарно-гладких нанокристаллов использовалась размерная зависимость физического свойства. Для предела текучести атомарно-гладких нанокристаллов нами получено уравнение, которое по форме совпадает с уравнением Холла – Петча. Однако коэффициенты пропорциональности в обеих формулах различаются. В рассматриваемом случае поведение предела текучести атомарно-гладких нанокристаллов определяется также величиной их поверхностного натяжения. Если в полученном уравнении для поверхностного натяжения учесть формулу Русанова А.И., то мы получим обратный эффект Холла-Петча.

Таким образом, обратный эффект Холла – Петча обусловлен размерной зависимостью поверхностного натяжения атомарно-гладких нанокристаллов и в конце концов зависит от атомного радиуса, который определяет толщину поверхностного слоя наноструктуры.

ABSTRACT

To date, the empirical Hall-Petch law and its inverse effect have been debated. Numerous models have been proposed and the inexhaustibility of the deep Hall – Petch concept has been shown. In the framework of this work, we want to show that the inverse Hall-Petch effect is observed not only in polycrystals, but also inherent in