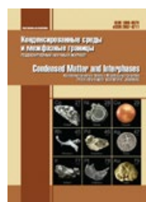

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Statistical approach to the process of tunnel ionisation of impurity centres near the heterointerface

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Abstract

To date, the processes of tunnel ionisation of impurities near the interface between two different semiconductors have been comprehensively studied. The most important parameters of the contact electron states of impurities have been determined. However, the calculated expressions for these parameters have been of local nature, as applied to individual impurities. Meanwhile, it is easy to understand that a number of processes, such as the flow of charge carriers and their diffusion through a heterojunction, are clearly statistical in nature. The same applies to the processes of tunnel ionisation of shallow and/or deep impurities near the interface. A statistical approach to the calculation of the parameters of tunnel ionisation of impurities broadens the opportunities for obtaining fundamental information regarding surface electron states.

The aim of this work was to use a statistical approach to study the effect of the heterointerface on the energy spectrum of shallow and deep centres. For this purpose, the expansion of the reflected quasi-classical wave function within the complete system of spherical harmonics and the subsequent extraction of the zero harmonic amplitude (*s*-component) was used to estimate the minimum distance from the impurity to the heterobarrier and to specify the limitations of the applicability of the results obtained in other works. The article analyses the conditions of the quasi-classical approximation which are used to estimate the order of the value for the minimum height of the potential barrier (pit).

This work (with due consideration given to the minimum distance estimate) presents averaged formulas obtained for the energy shift of the ground state and the lifetime of the quasi-stationary state depending on the distance from the heterobarrier. Some qualitatively new considerations can also be found in the article. The distribution of impurity centres near the heterobarrier is assumed to be uniform. The article discusses the role of electron transitions in causing the buffer field effect for both shallow and deep centres. The focus of the article is on the estimates of various physical parameters characterising electron transitions near the heterobarrier.

Keywords: Heterobarrier, Tunnelling, Shallow and deep centres, Energy shift of the ground state, Lifetime

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1. Introduction

The quasi-classical theory of tunnel ionisation of neutral impurity centres near the heterobarrier was constructed in [1–4]. However, in these studies, the calculation of the main parameters of metastable states (energy shift of the ground state and lifetime) of the impurity is of local nature and does not include many impurities concentrated near the heterojunction. To clarify the limitations of applicability of the obtained results [1], it is necessary to take into account the accumulation of shallow and/or deep neutral impurities near the heterojunction.

Various aspects of the reflection above a barrier and the tunnelling of charge carriers from the wide band-gap of the heterojunction to the narrow band-gap were considered in [2]. In this case, an electron from a donor centre located, for example, in the wide band-gap of the heterojunction, can tunnel through the potential barrier into the narrow band-gap of the heterojunction with a subsequent recombination with a hole. An excess of energy manifests itself in the bulk luminescence spectrum [5]. Taking into account the band discontinuity, an electron which was initially in a quasi-bound state changes into a quasi-free state. At the same time, the energy remains unchanged.

In [3, 4], a quasi-classical theory of ionisation of impurity centres under the action of external electric fields was constructed. The main results were obtained by the imaginary time method.

The main theoretical achievement of work [1] was the extraction of *s*, the component of the reflected quasi-classical wave function within the limit of a large ratio of distance L from the impurity centre to the heterobarrier to the effective Bohr radius of a shallow impurity ($L/r_B \gg 1$). As a result, the authors of [1] obtained an asymptotic formula for the energy shift of the ground state of a shallow impurity:

$$\delta E_B = -G(V_\circ)\frac{2L}{r_B}\exp\left(-\frac{2L}{r_B}\right)\cdot E_B, \qquad (1)$$

where $G(V_\circ) = \dfrac{\sqrt{E_B} - \sqrt{V_\circ + E_B}}{\sqrt{E_B} + \sqrt{V_\circ + E_B}}$ is the coefficient that determines the condition for the reflection of the wave function, E_B is the binding energy of a shallow impurity, and $V_\circ$ is the height (depth) of the heterobarrier.

However, the procedure for the extraction of the *s* component given in [1] does not allow indicating the threshold distance $L_{\min}$ from the centre starting from which the asymptotic formulas obtained in [1], and formula (1) in particular, would be effective for finding the energy shift of the ground state of a shallow and/or deep impurity.

Defining the $L_{\min}$ parameter is relevant if we take into account the fact that the condition of the quasi-classical approximation can be affected near the impurity [6]. The $L_{\min}$ parameter sets the "lower limitation" of the applicability of the theory developed in [1] and consequently the optimal distance from the accumulation of neutral impurities to the heterobarrier. As a consequence, formula (1) must have the $L_{\min}$ parameter.

The purpose of this study was to find the $L_{\min}$ parameter and to use it to obtain (taking into account the results of [1]) averaged formulas for the energy shift of the impurity state and lifetime of the quasi-stationary state depending on the parameter $L_{\min}$.

2. Calculation methodology

Mathematically correct extraction of the *s* component of the reflected quasi-classical wave function

$$\psi_+(\theta, L) = \frac{1}{\sqrt{\pi r_B^3}} G(V_\circ)\exp\left(-\frac{2L}{r_B\cos\theta}\right)\exp\left(\frac{L}{r_B}\right),$$

$$(0 \le \theta \le \pi/2) \qquad (2)$$

(if we expand $\cos\theta \approx 1 - \theta^2/2$ in formula (2), where θ is the angle of the wave incidence (reflection), we will end up with an approximate formula from work [1]) means the expansion of function (2) within the full system of spherical harmonics with a subsequent extraction of the zero harmonic amplitude:

$$\psi_+(\theta, L) = \sum_{l,m} a_{lm} Y_{lm}(\theta, \varphi). \qquad (3)$$

The a_{lm} coefficients are determined by the formulas:

$$a_{lm} = \int Y_{lm}^*(\theta, \varphi)\psi_+(\theta, L)\, d\Omega. \qquad (4)$$

For the zero harmonic coefficient:

$$a_{00}=\int Y_{00}^{*}(\theta,\varphi)\psi_{+}(\theta,L)\,d\Omega=$$
$$=\frac{1}{\sqrt{4\pi}}\frac{1}{\sqrt{\pi r_B^3}}G(V_\circ)\exp\left(\frac{L}{r_B}\right)\int_0^{2\pi}d\varphi\int_0^{\pi/2}\exp\left(-\frac{2L}{r_B\cos\theta}\right)\sin\theta\,d\theta=$$
$$=\frac{1}{\sqrt{r_B^3}}G(V_\circ)\exp\left(\frac{L}{r_B}\right)\int_0^{\pi/2}\exp\left(-\frac{2L}{r_B\cos\theta}\right)\sin\theta\,d\theta=$$
$$=\frac{1}{\sqrt{r_B^3}}G(V_\circ)\exp\left(-\frac{L}{r_B}\right)\left\{1-\frac{2L}{r_B}\exp\left(\frac{2L}{r_B}\right)\left[-\mathrm{Ei}\left(-\frac{2L}{r_B}\right)\right]\right\}, \quad (5)$$

where $-\mathrm{Ei}(-z)$ is integral exponent [7].

At $2L/r_B \gg 1$, from expression (5) it follows:

$$a_{00}\approx\frac{G(V_\circ)}{2L\sqrt{r_B}}\exp\left(-\frac{L}{r_B}\right). \quad (6)$$

Substitution of (6) into expansion (3) gives the zero harmonic amplitude:

$$\psi_{+}(\theta,L)\approx a_{00}\cdot Y_{00}\approx\frac{G(V_\circ)}{2L\sqrt{r_B}}\exp\left(-\frac{L}{r_B}\right)\cdot\frac{1}{\sqrt{4\pi}}=$$
$$=\frac{G(V_\circ)}{4L\sqrt{\pi r_B}}\exp\left(-\frac{L}{r_B}\right). \quad (7)$$

As can be seen from (7), the asymptotic behaviour of the *s*-component of function (2) corresponds to the asymptotic behaviour obtained in [1]. Numerical calculations of function $\Phi(z)=1-z\exp(z)[-\mathrm{Ei}(-z)]$ from expression (5) show (Table) that the transition to the asymptotic formulas in [1] begins approximately from the distance $L_{\min}\approx 5r_B$ and in this context:

$$\Phi(z)=\begin{cases}1-z\exp(z)[-\mathrm{Ei}(-z)], & (z<10)\\ 1/z, & (z\ge 10)\end{cases}. \quad (8)$$

At distances shorter than $L_{\min}\approx 5r_B$, the theory developed by the authors of [1] cannot properly explain the experimental results of [2, 5] and is rather a rough approximation.

To calculate the energy shift per unit of distance, for simplicity, we will assume that the distribution of impurity atoms over the matrix volume near the heterojunction is uniform and isotropic.

$$\overline{\delta E_B}=\lim_{L\to\infty}\frac{1}{\Delta L}\int_{L_{\min}}^{L}\delta E_B(x)dx=\frac{1}{\Delta L}\int_{L_{\min}}^{\infty}\delta E_B(x)dx. \quad (9)$$

By substituting formula (1) in expression (9) (we assume that the value L is a variable) we get:

Table. Values of the F(z) function

z	5	10	15	20
$\Phi(z)$	0.15	0.09	0.07	0.05

$$\overline{\delta E_B}=-G(V_\circ)\left(1+\frac{2L_{\min}}{r_B}\right)\frac{r_B}{2\Delta L}\exp\left(-\frac{2L_{\min}}{r_B}\right)\cdot E_B. \quad (10)$$

Accordingly, for the average lifetime of an electron at $V_\circ<-E_B$:

$$\overline{\tau_B}=\frac{\hbar}{2E_B}\frac{|V_\circ|}{\sqrt{E_B\left(|V_\circ|-E_B\right)}}\frac{\Delta L}{r_B}\frac{\exp(2L_{\min}/r_B)}{1+2L_{\min}/r_B}. \quad (11)$$

This time is minimal if $V_\circ=-2E_B$.

Here, ΔL characterises the effective size of the impurity layer near the heterojunction (Fig. 1). As the electrons move from impurity levels to a free state, the layer becomes positively charged and acquires the character of a buffer electric field, which, however, does not have a significant effect on the tunnelling effect. The value of ΔL cannot significantly exceed r_B (~ 10 Å). At the same time, ΔL cannot be less than the critical distance between atoms ($\Delta L\ge 4r_B$) (Mott's transition) [8]. For estimates, you can assume that $\Delta L\approx L_{\min}\approx 5r_B$. For a model semiconductor with the parameters of $E_B=0.01$ eV and $V_\circ=0.1-1$ eV, the estimate for the lifetime of the bound electron according to formula (11) gives a value of the order of $5\cdot 10^{-10}$ s. Using $L_{\min}\approx 5r_B$ the criterion of quasi-classical behaviour ($\lambda\!\!\!^{-}<L_{\min}$) can be determined:

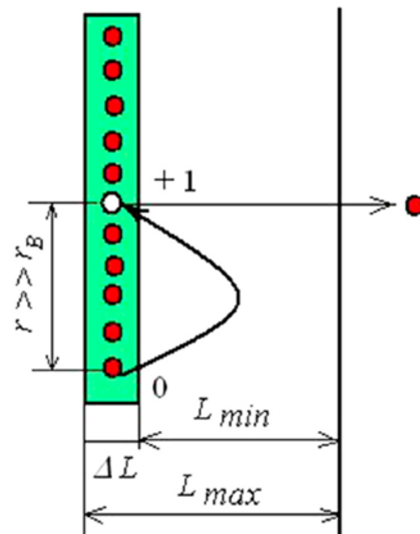

Fig. 1. Scheme of electronic transitions near the heterojunction

$|V_\circ| > 1.04 E_B$. (12)

Consequently, when $|V_\circ| = 1.04 E_B$, the condition of applicability of the quasi-classical approximation, i.e. the heterobarrier, must be sufficiently high (deep). By further developing this line of reasoning, it is possible to interpret $\overline{\delta E_B}$ as the average energy of shift of the ground state of impurity atoms within the effective width ΔL obtained from the beam of quasi-classical electrons. The estimation of $\overline{\delta E_B}$ by formula (10) for a model semiconductor is approximately 10^{-5} eV. The energy shift of the ground state of impurity (10) cannot be less than the value of its natural width (10^{-7} eV). This imposes certain limitations on the value of L, namely $L_{max} < 10\, r_B$. In case of great distances, formula (10) gives unrealistically low values for $\overline{\delta E_B}$. To compare, for example, the binding energy of $D^-(A^+)$ centres is of the order of meV [9].

It is interesting to compare the lifetime of a bound electron in relation to its changing into a free state with its tunnelling time between small impurities (Fig. 1). The theory provides the following formula for the tunnelling time between the centres [6]:

$$\overline{\tau_{0\to1^+}} = \frac{\pi\hbar}{\overline{\delta E_{0\to1^+}}}, \quad (13)$$

and

$$\overline{\delta E_{0\to1^+}} \approx \frac{8r}{3r_B}\exp\left(-\frac{r}{r_B}\right)\cdot E_B, \quad (14)$$

where r is the average distance between the impurity atoms.

At concentrations of shallow impurities of 10^{18} cm^{-3}, formula (14) gives a value of $1.2\cdot10^{-5}$ eV, almost equal to $\overline{\delta E_B}$, i.e. $\overline{\tau_B}/\overline{\tau_{0\to1^+}} \approx 3$. This means that for highly doped semiconductors at very low temperatures (about 2–4 K), there is hardly any effect of the buffer (quasi-electric) field and in general the impurity layer ΔL is quasi-neutral. The quasi-neutral behaviour of the layer can be disturbed by exposure to radiation, heat treatment, etching, application of an external electric field, etc. [10].

In case of the deep centre described by the "zero" radius potential [1] within the framework of this model, the bound electron has no excited states and has one single bound state. This allows considering the amplitude of the "zero harmonic" of decomposition (3), which is the only one of its kind [9]. Calculations similar to the ones used to derive formula (7) give the following formula for the amplitude of the zero harmonic of the reflected quasi-classical wave function:

$$\psi_+(\theta, L) = \frac{A(V_\circ)}{8L^2}\sqrt{\frac{a_\circ}{\pi}}\exp\left(-\frac{L}{a_\circ}\right) \quad (2L/a_\circ \gg 1), \quad (15)$$

where $A(V_\circ) = \dfrac{\sqrt{E_\circ} - \sqrt{V_\circ + E_\circ}}{\sqrt{E_\circ} + \sqrt{V_\circ + E_\circ}}$, $a_\circ = \hbar / \sqrt{2m^* E_\circ}$ are the size of the wave function of the electron bound at the deep centre ($a_\circ$ usually does not exceed several constant lattice spacings [11]), m^* is the effective mass of the electron, and $E_\circ$ is the binding energy of the electron at the deep centre (of the order of eV).

Considering the fact that function (8) is universal, it is possible to immediately specify the lower limitation of the applicability of formula (15): $L_{\min} \approx 5a_\circ$. By averaging the formula for the energy shift of the deep state obtained in work [1]:

$$\delta E_\circ = -A(V_\circ)\frac{a_\circ}{L}\exp\left(-\frac{2L}{a_\circ}\right)\cdot E_\circ \quad (16)$$

and using expression (9), we have:

$$\overline{\delta E_\circ} = -A(V_\circ)\frac{a_\circ}{\Delta L}\left[-\mathrm{Ei}\left(-\frac{2L_{\min}}{a_\circ}\right)\right]\cdot E_\circ$$

$(\Delta L \approx L_{\min})$. (17)

From (17) the approximate formula follows:

$$\overline{\delta E_\circ} \approx -A(V_\circ)\frac{a_\circ}{10L_{\min}}\exp\left(-\frac{2L_{\min}}{a_\circ}\right)\cdot E_\circ$$

$(L_{\min} \approx 5a_\circ)$. (18)

Accordingly, the average lifetime of an electron at the deep centre when $V_\circ < -E_\circ$:

$$\overline{\tau_\circ} = \frac{5\hbar}{2E_\circ}\frac{|V_\circ|}{\sqrt{E_\circ(|V_\circ| - E_\circ)}}\frac{L_{\min}}{a_\circ}\exp\left(\frac{2L_{\min}}{a_\circ}\right). \quad (19)$$

By comparing (11) and (19) we can conclude that heterobarrier affects the position of the shallow impurity more (by about 30 times). It is clear that screening greatly reduces the probability of an electron jumping from a neutral impurity to an ionised (+1) impurity. The time required

to neutralise the deep impurity significantly exceeds the lifetime of the bound electron of the shallow impurity, and the buffer field effect will be observed for a long time. At the same time, electronic transitions between deep and shallow centres are quite possible. The corresponding calculations are described in [12–17].

3. Discussing the results with regard to the AlGaAs/GaAs heterostructure

Let us discuss the conditions for the applicability of the obtained formulas in relation to a specific AlGaAs/GaAs heterostructure with a deep centre (Fig. 2). The forbidden energy gap of gallium arsenide is 1.5 eV and in a solid solution of $Al_xGa_{1-x}As$ it increases with the growth of x. For example, at x = 1, the forbidden energy gap in the AlAs compound is 2.2 eV. As we noted above, the buffer field effect (developed within the framework of the statistical approach) will work for a long time in the case of a deep centre. Let us estimate the minimum buffer field value for the DX centre in AlGaAs. Assuming $|V_0| = 0.75$ eV, $E_0 = 0.7$ eV (Fig. 2), we will find (e-charge of the electron):

$$\mathrm{E}_{\mathrm{buff}} = \frac{|V_\circ| - E_\circ}{eL_{\min}} \approx 2.4 \cdot 10^2 \text{ V/cm}$$
$$(|V_\circ| - E_\circ << E_{\mathrm{opt}}). \tag{20}$$

Indeed, as we can see, the intensity of the buffer field is much less than the intensity of the optical ionisation field of the DX centre ($E_{\mathrm{opt}} \approx 1.3$ eV) [18].

Also, we would like to note that the basic value of $L_{\min}$, which we operated on with within the framework of the statistical approach, coincides with the critical distance from [18] ($L \approx 70$ Å). In general, all this confirms the correctness of the initial formulas (10), (11), (18), and (19).

Therefore, the statistical approach to tunnel ionisation of deep centres leads to approximately the same results as the multiphonon mechanism of ionisation of DX centre in heterostructures [18].

4. Conclusions

The content of the work can be summarised by formulas (10), (11), (18), and (19), which clarify the relevant formulas obtained in the work [1]. Numeric evaluations (Table) indicate that there is a well-defined distance from the impurity centre $L_{\min} \approx 5r_B$ ($L_{\min} \approx 5a_\circ$) to the heterobarrier,

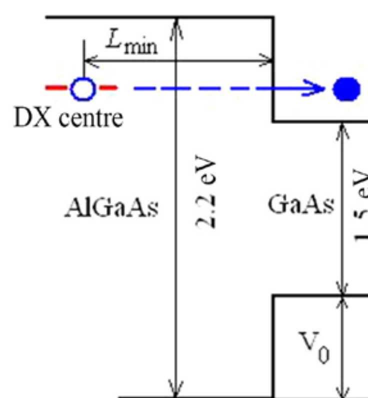

Fig. 2. First-order heterojunction (AlGaAs/GaAs). Specified tunnel transition of the electron from the DX centre

starting from which the asymptotic formulas obtained in [1] are quite accurate. This applies equally to formulas (10), (11), (18), and (19) derived from these asymptotic behaviours. After being averaged, formulas (1) and (16) of Efros et al. became a statistical average of (10) and (18). From formulas (10) and (18), it follows that the greatest contribution to the total energy shift is provided by impurity centres localised at a distance of $L = L_{\min}$ from the heterointerface. This fact is not mentioned in the asymptotic formulas of Efros et al. In addition, the formulas of Efros et al. do not allow developing the idea of the "buffer field" effect, which is purely statistical in nature.

The "buffer field" effect is produced in the case of deep impurities [18]. Then, there is some similarity with quasi-electric fields in variband semiconductors. For shallow impurities, in this situation, this effect is never produced.

Conflict of interests

The author declares that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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