Change in the ionization energy of impurities as a result of wave function relocation in a system of quantum wells

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The change occurring in the binding energy of the electrons on impurity atoms as a result of the relocation of the wave function in a system of quantum wells in an external electric field, which is longitudinal with respect to the axis of growth of the heterostructure, was investigated. As a result of this effect, the concentration of free charge carriers changes substantially and the lateral conductivity of the system is thereby modulated. © *1995 American Institute of Physics.*

1. Relocation of the electronic wave functions,[1] which occurs in a system of quantum wells under the action of an external electric or magnetic fields,[2] electromagnetic radiation,[3] or temperature,[4] can be used as a basic concept for the development of a new class of fast quantum devices.[5]

One application of this concept is modulation of the lateral (along the layers) conductivity of a system of quantum wells (QWs) by an external electric field which is oriented parallel to the axis of growth of the heterostructure (HS). As a result of the relocation, occurring in an external field, of the maximum of the modulus of the electronic wave function from a low-mobility quantum well into a high-mobility well (the corresponding values can increase by more than an order of magnitude), the total conductivity of the system also increases. The idea of a mobility-modulated, field-effect transistor was proposed previously in a classical variant by Sakaki[6] and was later perfected in Ref. 7, taking into account quantum effects. However, this idea has still not found any practical applications because of the low degree of modulation of the conductivity of the system.

In the present paper we investigate the change occurring in the ionization energy of impurity atoms as a result of the relocation of the electronic wave function in a system of quantum wells. This effect has never before been mentioned by anyone. Besides being of interest in itself, it is also of interest because it offers the possibility of increasing by several orders of magnitude the degree of modulation of the lateral conductivity of a system of quantum wells (employed, for example, as a channel in a field-effect transistor)

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by using the external electric field to change the electron mobility and the electron concentration.

2. The effect of relocation of an electronic wave function on the ionization energy of an impurity atom can be monitored by using the effective-mass method. The Schrödinger equation for the envelope function $\Phi(\mathbf{r},z)$ of the electronic wave function has the form

$$\left\{-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial \mathbf{r}^2}+\frac{\partial^2}{\partial z^2}\right)+U(z)-eFz+V(\mathbf{r},z)\right\}\Phi(\mathbf{r},z)=E\Phi(\mathbf{r},z), \tag{1}$$

where e and m are, respectively, the charge and effective mass of an electron; $U(z)$ is the initial potential of the heterostructure; $V(\mathbf{r},z)$ is the potential produced by an impurity atom; and, F is the intensity of the electric field. The z axis is directed along the axis of growth of the heterostructure and $\mathbf{r}=(x,y)$. The effective mass m of an electron is assumed to be isotropic. The differences in the effective masses in the materials of the quantum wells and the barriers as well as the relatively weak nonparabolicity of the conduction band are not important for the quasimomenta studied in this problem.

It is convenient to represent the envelope of the wave function of an electron localized on an impurity as an expansion in a system of the eigenfunctions of Eq. (1) without the impurity potential. These functions can be written in the form

$$\varphi_{n\mathbf{k}}(\mathbf{r},z;F)=S^{-1/2}\psi_n(z;F)e^{i\mathbf{kr}}, \tag{2}$$

where S is the normalizing area (in the xy plane), $\psi_n(z;F)$ is a one-dimensional envelope function, n is the number of the quantum-well subband, and $\mathbf{k}$ is the quasimomentum of free motion in the xy plane. In writing expression (2) we took into account the fact that the dependence of the envelope functions on the quasimomentum can be ignored for the relatively small values of $\mathbf{k}$ which are of interest.

An electric field applied along the axis of the heterostructure makes the quantum-size states of the electrons quasistationary. For the lower subbands and relatively weak fields the characteristic decay times of such states are long—an estimate shows that such states can be regarded as being stationary, if

$$F \ll m^{1/2}E^{3/2}/\hbar e. \tag{3}$$

Here E is the electron energy measured from the bottom of a quantum well. In the case of nanostructures $F \ll 10^6$ V/cm.

We consider the case of a strongly localized impurity potential, which we represent in the form

$$V(\mathbf{r},z)=-V_0 a^3 \delta(\mathbf{r})\delta(z-z_0). \tag{4}$$

Here z_0 is the coordinate of the impurity atom, and V_0 is the depth of the potential well. To preserve the required dimensions, the lattice parameter a is included in the definition of $V(\mathbf{r},z)$. The potential (4) describes well the characteristics of deep levels in semiconductors. We also note that the long-range part of the impurity potential in highly doped structures is effectively screened.

Lifshitz's equation[8] which determines the energy of a localized electronic state, for the potential (4) can be represented in the form

$$\frac{V_0 a^3}{(2\pi)^2}\sum_n \left\{ |\psi_n(z_0;F)|^2 \int \frac{d^2\mathbf{k}}{E_n(\mathbf{k})+E_{\text{imp}}} \right\} = 1. \tag{5}$$

Here E_{imp} is the binding energy of an electron on an impurity center. If only the bottom subband is taken into account, then the following analytic expression can be derived for the binding energy:

$$E_{\text{imp}}(F) = \frac{\pi^2\hbar^2}{2ma^2}\left[\exp\left(\frac{2}{wa|\psi_1(z_0;F)|^2}\right) - 1\right]^{-1}, \tag{6}$$

where the dimensionless parameter $w = ma^2V_0/\pi\hbar^2$ can be regarded as the effective strength of the impurity potential. The factor $|\psi_1(z_0;F)|^2$, which depends on both the position of the impurity in the heterostructure and on the electric field, causes the binding energy to depend strongly on the field.

In what follows we restrict the analysis to a system of two quantum wells. We take into account the two bottom quantum-well subbands, since in the nanostructures of interest to us with two quantum wells the higher subbands of the conduction band (if they arise at all) lie far above the first two subbands. The splitting between the first two subbands is generally comparable to the binding energy of an electron in an impurity state.

When the wave function corresponding to the bottom subband is relocated from one quantum well into another, the wave functions of the other subbands are also relocated, and since the wave functions remain orthogonal, the probability density in these subbands is redistributed in opposite directions. For example, when the first envelope is transferred from a wider into a narrower quantum well, the second envelope is found to be localized mainly in the wider quantum well. Of course, the second quantum well in this case can strongly influence the binding energy of the impurity state.

When two or more subbands are taken into account, a simple analytic solution of the type (6) for the binding energy cannot be obtained, and the Eq. (6) must be solved numerically. In so doing, it is necessary to determine the value of the parameter w, which can be found if the three-dimensional binding energy $E_{\text{imp}}^{(3D)}$ for the given impurity is known. In this case Eq. (5) gives $w = 1/(1-\xi\tan^{-1}\xi)$, where $\xi = (2ma^2E_{\text{imp}}^{(3D)}/\pi^2\hbar^2)^{1/2}$. The parameter w can also be calibrated from the experimentally measured value of the binding energy of an impurity state in a heterostructure with a single quantum well of appropriate width.

3. We now consider the possible manifestations of the effect. The lateral conductivity of the system of quantum wells

$$\sigma = -\frac{e^2}{2\pi\hbar^2}\sum_n \int E\tau_n(E)\frac{\partial f(E)}{\partial E}\,dE \tag{7}$$

depends on two parameters: the relaxation time $\tau_n(E)$ and the Fermi energy via the quasi-Fermi electron distribution function $f(E)$. By producing with an electric field a relocation of the wave function from one quantum well into another we can influence both of these parameters and thereby control the conductivity of the system.

The inverse relaxation time can be represented as a sum of the reciprocals of the partial times

$$\tau_n^{-1}(E)=\sum_m \tau_{nm}^{-1}(E) \tag{8}$$

and is determined by intrasubband ($n=m$) and intersubband ($n \neq m$) scattering processes. The intersubband scattering processes predominate in a relatively narrow range of electric fields, where the maximum overlapping of the envelope functions of different energy subbands is obtained in the relocation process.

In the case of scattering by the potential (4) we obtain

$$\tau_{nm}^{-1}(E)=\frac{(V_0a^2)^2}{\hbar}\int_0^{\infty} kdk\,\delta(E_n(k)-E_m(k))\int_{-\infty}^{\infty} dzN(z)\psi_n^2(z)\psi_m^2(z), \tag{9}$$

where $N(z)$ is the distribution of the impurity in the sample. If only one quantum well is doped, then in the case where the wave function is redislocated by a field into the other quantum well, the value of the last integral on the right-hand side of Eq. (9) decreases as a result of the decrease in the degree of overlapping of the functions $N(z)$ and $\psi_n(z)$. As a result, the relaxation time and the conductivity of the system increase. The operation of field-effect transistors is based on this principle.[6,7] When we act on the ionization energy E_{imp} of the impurities by relocation of the wave function, we also control the position of the quasifermi level and therefore the concentration of the current carriers. The effect of this factor can be much greater than that of selective scattering, and combined they can give a high degree of modulation of the lateral conductivity of the system.

4. To illustrate the arguments presented above, we solved Lifshitz's equation (5) numerically for a number of specific structures of the type $Al_xGa_{1-x}As/GaAs$, containing two, three, and more quantum wells. We found the envelope functions and the energies of the subbands from Schrödinger's equation (1) with $V(\mathbf{r},z)\equiv 0$. When necessary,[4] the Coulomb interaction was taken into account by solving Poisson's equation self-consistently.

We present below the most characteristic results obtained for the structure 9–7–7, where the numbers indicate the width of the first quantum well, the width of the internal barrier, and the width of the second quantum well, respectively, in units of the interatomic distance (we used the value $a=5.665\times 10^{-8}$ cm). The depth of the quantum wells is 0.3 eV. It was assumed that the impurity is located at the center of the wider quantum well. The initial donor-impurity ionization energies required for determining the parameter V_0 were assumed to be 20 meV for Si-type impurity and 100 meV for the deeper impurity Te in a GaAs quantum well with a width of 10 interatomic spacings. The computational results for the binding energy plotted as a function of the strength F of the electric field are shown in Fig. 1. Two size-quantization subbands were taken into account in the calculation. The cases where $E_{\text{imp}}<\Delta$ (curve 2) and $E_{\text{imp}}>\Delta$ (curve *3*), where Δ is the distance between the extrema of the subbands for $F=0$, were considered. For comparison, the function $E_{\text{imp}}(z_0;F)$, calculated taking into account only the bottom subband

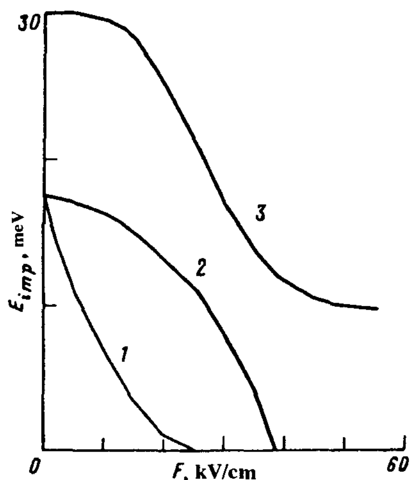

FIG. 1. Ionization energy of an impurity Si atom in a test structure with two quantum wells as a function of the applied electric field. The curve *1* corresponds to the case $E_{\text{imp}}(0)<\Delta(0)$ with only the bottom subband taken into account. The curves *2* and *3* were calculated taking into account the contributions of two quantum-well subbands with $E_{\text{imp}}(0)<\Delta(0)$ and $E_{\text{imp}}(0)>\Delta(0)$, respectively.

(curve *1*), is also shown in the same figure. Many asymmetric nanostructures with two and more quantum wells exhibit a similar behavior of the binding energy with increasing field.

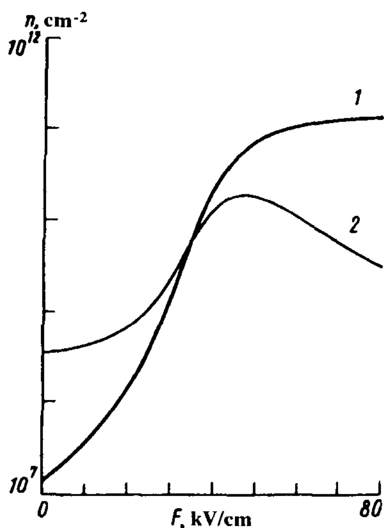

FIG. 2. Surface electron concentrations (on a logarithmic scale) in different quantum wells of a two-well test structure, selectively doped with Te impurity, as a function of the applied electric field at $T=77$ K: *1*—Quantum well with low electron mobility and *2*—quantum well with high electron mobility.

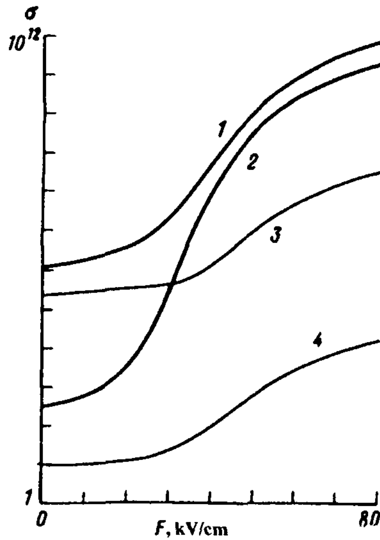

FIG. 3. Lateral conductivity of a test structure with two quantum wells, one of which is doped, as a function of the applied electric field (in relative units on a logarithmic scale). The curves correspond to the following cases: *1*—Si impurity at $T=10$ K, *2*—Te impurity at $T=77$ K; *3*, *4*—same but the change in the ionization energy is ignored.

The external-electric-field dependence of the surface electron concentration (on a logarithmic scale) in different quantum wells of a two-well test structure with Te impurity is shown in Fig. 2. It follows from this figure that at a temperature of 77 K (for which the calculation was performed) the change in the concentration as a result of the relocation of the wave functions can amount to several orders of magnitude.

The lateral conductivity of the two-well test structure was calculated using Eq. (7) and the previously determined envelope wave functions. The position of the Fermi level was determined by direct calculation of the number of particles in the system under the condition that the electron distribution function has the Fermi form. The volume concentration of the donor impurity in the wider quantum well was assumed to be 10^{18} cm^{-3}. Uniformly distributed uncontrollable acceptor centers with a volume concentration of 10^{14} cm^{-3} were assumed to be present in the structure. The dependence of the lateral conductivity of the test structure (on a logarithmic scale in relative units) as a function of the applied electric field with a wide quantum well doped with shallow donor impurities Si or Te is shown in Fig. 3. The thick curves *1* and *2* were calculated taking into account the change produced in the ionization energy of the impurity atoms in an external field by the relocation of the wave function from the quantum well with low electron mobility into the quantum well with high electron mobility. The thin curves *3* and *4* were computed ignoring this effect.

The high degree of modulation of the lateral conductivity of the system of quantum wells in an external electric field (compared to the results of Refs. 6 and 7) makes the effect studied in this work useful for a new-generation of quantum devices.

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