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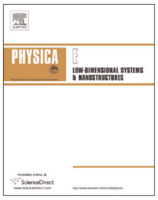

On some new effects in delta-doped QWs

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HIGHLIGHTS

- We describe new phenomenon connected to ionization of impurity delta layer within QW.
- It leads to the increase of impurity binding energy.
- Effect of distribution model of the impurity within delta-layer is negligible.
- Ionization leads to a change of energy separation between energy levels in the QW.
- The idea of an optical modulator controlled by a weak electric field is put forward.

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ABSTRACT

Self-consistent calculation of Schrodinger, Poisson and electroneutrality equation with embedded impurity binding energy calculations of delta-doped SiGe/Si quantum well structures are performed. The influence of several parameters of the structure on the impurity binding energy is studied and discussed. On the basis of found phenomena the idea of an optical modulator controlled by a weak electric field is put forward.

1. Introduction

Doping has always been among the most important issues in semiconductor physics as it determines the main characteristics of a great majority of semiconductor devices. The developing of nanotechnologies [here and after we will only refer about the particular case of rectangular semiconductor quantum wells (QWs)] has led to some shift of accents in the study of impurity-related properties. The attention was, first of all, focused on achieving an increase of the charge carrier mobility and it was the reason for the search of ways to remove impurities from the QWs. Outstanding milestones along the way were modulation doping [1] and barrier delta-doping processes [2], which made possible to combine the high carrier concentration of electrons in such QWs with their high mobility. On the other hand, the appearance of a big oscillator strength for intersubband optical transitions allowed one to use those structures both to generate the emission of radiation (e.g. quantum cascade lasers [3]), and for serving as quantum well infrared photodetectors (QWIP, [4]). Once again, in spite of the fact that active QWs are sometimes (heavily) doped, the impurities, nevertheless, play an auxiliary role in these structures. Therefore one may conclude that, up to now, there are not yet any actual device based on impurity properties in QWs. In fact, impurities in a QW are very interesting objects of study. The point is that the impurity binding energy (IBE) is very sensitive to the

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variation of practically all the parameters of the QW. At this point, it is worth to recall here a work by Bastard, published more than thirty years ago [5]. In that work he considered the case of infinitely deep QWs and showed that IBE depended on the width of the well as well as on impurity position inside the well.[1] Since then, researchers have proven the IBE dependence on the QW's depth and width [6–8], the width of the barriers for multi-QW structures [9], nonparabolicity of the dispersion low in the space-quantized subbands [10], difference in the effective masses in well and barrier regions [7], dielectric constant mismatch between the barrier and well materials [11], and screening by free electrons [12,13]. In addition, the effect of all thinkable external influences on the IBE such as: electric and magnetic fields and uniaxial strain [14–22], hydrostatic pressure [23–25], and the intensity of powerful laser radiation [26–29] have also been in the focus of research for some time. Also, the effect of temperature was analyzed by using the Schrodinger equation with temperature-dependent electron effective masses, dielectric constants and well depth [30–32]. In all these works it was supposed that IBE does really exist. In other words, an assumption of a single impurity located at different places within a QW was used. But nowadays we know about the possibility of using modern nanotechnologies to create an ordered distribution of impurities in QW systems. Here we shall specifically take into account the impurity delta-doping in QWs. And it turns out that ionization of impurities in the delta-layer leads to some new phenomena. Indeed, the joint potential of ionized impurities and free electrons in the QW creates an additional electrostatic potential (we will call it the Hartree potential), which overlaps the original (rectangular) QW energy profile. As a result, one has a new QW with a new structure of dimensional quantization levels and, accordingly, with new IBE in the delta-layer. The fact that such a considered picture is not fictional was shown in our previous works [33,34], for a homogeneous distribution of impurities along the width of the delta layer. Let us note the main conclusions of those works. First, the IBE in the delta layer significantly depends (increases) on the degree of ionization of the delta layer. And most notably, it is seen for the case of edge-doped QWs. Secondly, one gets the ability to control energy separation between space-quantized levels due to ionization of the delta layer. Since we consider these findings to be important, the aim of this work is to make a further study of the mentioned phenomena. As in the works [33,34] the temperature is used for inducing the ionization of the delta-doping layer, although one can bear in mind that it can also be easily done by applying a relatively small electric field. We also go on with explanations for the approaches used in our works and present some new, unpublished, results on the subject. Accordingly, the work is organized as follows: Section 2 is preliminary. It provides a rationale for the chosen structure of research; considers the range of impurity concentrations within which the examined effects can be seen, and justifies approaches we use in writing the model Hamiltonian of the problem. Section 3 is devoted to describing the technique of finding a self-consistent solution of the Schrödinger, Poisson and electroneutrality equations. In Section 4 we present and discuss the obtained results and Section 5, with the main conclusions of the present work, closes the article.

2. Preliminary remarks

2.1. Model

As a model we use n-type, phosphorus-delta-doped $Si_{0.8}Ge_{0.2}/Si/Si_{0.8}Ge_{0.2}$ QW with infinite long barriers. It is supposed that the structure was grown along the [100] crystallographic direction, which is taken as the *z*-axis. Before proceeding to the justification of the kind of structure chosen for our research, we must highlight that the main results obtained in the previous works [33,34] – namely, that the ionization of the delta layer situated within a QW involves changes of both IBE and energy separation between space-quantized subbands; are particularly important for use of the so-called intracenter inversion mechanism in QWs. Initially, this mechanism was developed to explain the THz radiation from uniaxially compressed p-Ge in strong electric fields [35–37]. It is well known [38] that uniaxial pressure removes degeneration of both valence subbands at the Γ point of the reciprocal space and modifies (shallow) impurity states as well. At certain value of pressure the upper (we consider the energy of the valence subbands directed upward) split impurity level (attached to the second subband) may enter a continuous energy spectrum of the lower subband and thus become resonant [39]. Then, impurity states localized in the forbidden gap, are emptied by the applied electric field and holes appear in the lower subband. There they are accelerated by the same electric field and reach delocalized (resonance) impurity states and become captured by them [40–42]. Thus, inversion population of holes between delocalized and localized impurity states can occur in the THz range. It was also shown [41] that the most favourable conditions for the capture of charge carriers by resonant states occurs for an angle between electron wavevector and uniaxial pressure direction close to 90°. But this condition is automatically satisfied for the stressed QWs (due to lattice-constant mismatch between well and barrier materials). At the time, there were some reports about the generation of THz radiation from doped p-type SiGe QWs based on the intracenter inversion scheme [43,44] as well. It was emphasized in these papers that the essential feature of SiGe quantum wells used was that they were strained due to the lattice constant mismatch between the well and barrier materials. However, doped Si-based n-type QWs are also of interest, since the resonant impurity states are under each exited space-quantized energy level. And they are also stressed. Besides, the theoretical analysis of p-type structures is complicated by the complex structure of valence band. Thus, we decided to start studying impurity states for delta-doped n-type Si-based quantum wells. An important element is the fact that this kind of structures have also been carefully investigated just in the course of the development of the intracenter inversion theory [45]. It means that we have the additional possibility to compare our results with those of the work [45] where it is possible. And last but not least, the structure is Si-based, which means that a resulting prospective device would easily be consistent with well developed Si technology.

2.2. On the method and the central cell effect on IBE

We will look for obtaining the impurity binding energy in the framework of the effective mass approximation, which does not allow for central cell effect on (or chemical shift of) IBE. Nevertheless, after we get the IBE, we will take the chemical shift into account by following the method developed in the reference [45].

2.3. About constants and main assumptions

Effective masses and Bohr radii are important parameters in the justification of the used approximations. Their values are in

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[1] Cited in this part of literature reflects only authors′ choice and cannot be considered as complete and comprehensive.