WILEY-VCH

DOI: 10.1002/ ((please add manuscript number))
Article type: Full Paper

Toward Superlattices in 1D Quantum Wires

*Victor Petrov**
Institute of Radio Engineering and Electronics, Russian Academy of Sciences,
Moscow, 103907, Russia

*Corresponding author: Dr. Victor Petrov. e-mail: vpetrov@cplire.ru

Keywords: 1D quantum wires, superlattices, minigaps

As is well known, lateral superlattices on semiconductor vicinal planes are realized in 2D electron systems on high-index Miller surfaces. In this work we suggest a new method of development of vicinal superlattices in 1D quantum wires on semiconductor low-index surfaces. For this purpose we suggest to orient the axis of the wire at the necessary angles to the basic translation vectors on a low-index surface (for instance, in the MOS system with the use of a narrow gate). In this case in the quantum wire the new basic translation period along the axis of the wire $A >> a_0$ (a_0 - lattice constant) appears.

1. Introduction

It is well known that a number of the already existing and possible device applications in nanoelectronics is based on the use of various superlattice effects, i.e. the superlattices in such systems are base elements. At the present time the majority of experimental and theoretical investigations of superlattice effects are devoted, basically, to two types of superlattices. First of all, these are superlattices on a basis of multilayer structures with quantum wells on the basis of a combination of semiconductors with a different width of the forbidden bands (for example, the system GaAs - GaAlAs), the idea of which creation was offered by Esaki and Tsu [1]. At present, these superlattices are being investigated most intensively. The second system in which various superlattice effects were detected are superlattices in two-dimensional electron systems created near vicinal semiconductor heteroboundaries which are oriented on high-index Miller crystallographic planes. The possibility of existence of such

superlattices was predicted theoretically [2,3], simultaneously and independently they were realized [4]. Minigaps (MGs) in such a superlattice (further, it is simply referred to as the vicinal superlattice (VSL)) arise because of the appearance in a plane of a quantum well of a new basic translation period A> > a_0 (a_0 - lattice constant) which is determined by crystallographic orientation of heteroboundaries. A detailed description of such VSL is given in monograph [5]. For the first time minigaps in such VSL was experimentally detected in MOS structure on the basis of Si [6]. By the present time, most fully experimentally investigated are VSLs in MOS structures on the basis of Si and InSb (review articles [7,8]) and on vicinal GaAs surfaces in GaAs - GaAlAs systems [9,10]. However, by now all these VSLs have been investigated only in 2D systems. At the same time, it is known that superlattice effects should be maximal in quantum wires when the period A appears along the axis of the wires. At the present time, various effects in quantum wires were investigated.

2. Main results

In the present work we put two tasks. First, to present a new method of development of the VSL in quantum wires on semiconductor low-index surfaces. Second, to demonstrate that the accounting of only the crystal potential and potential locating a particle (even without the accounting for the periodic step structure on the boundaries of the VSL) already results in the occurrence of MGs in the energetic spectrum of the particles in such systems.

We will present a new method of development of the VSL in quantum wires. The special feature of this method is a combination of the main properties of the VSL - the separation in the system by some way of a long translation period A - with the possibility of developing this situation in the quantum wire on semiconductor low-index surfaces. It is easy to see that this situation is possible when the axis of the quantum wire which lies on the low - index surface will be oriented at the necessary angles to the basic translation vectors along the surface like **(Figure 1)**. In this case the translation symmetry of the quantum wire will be determined by its orientation on the crystal surface since the possibility of a free motion only

along the axis of the wire selects in the initial two-dimensional translation group along the surface a one - dimensional translation subgroup along the wire with the basic period A. Thus, in the two - dimensional VSL the period A along the surface is selected by the orientation of the high-index surface whereas in the one-dimensional VSL it is selected by the orientation of the wire on the low - index surface. For example, if the quantum wire is realized in the MOS system with the use of a narrow gate [11], then the orientation of the wire will be determined simply by the appropriate orientation of the gate. If for the formation of the channel δ-doping or the existence of p-п doping areas on the crystal surface are used, appropriate orientation of a line δ-doping or appropriate arrangement p and n areas are necessary.

Let us proceed to the consideration of the second task beginning from the question on the physical nature of MGs arising in vicinal superlattices. In the beginning, we shall present briefly the situation existing at the present time in the already realized VSLs in two-dimensional systems. In such VSL, as created in MOS structures near high-index surfaces and in quantum wells limited by two high-index heteroboundaries, for example, in the GaAs-GaAlAs system, in the ideal case on boundary (boundaries) VSL there is a periodic step structure of atomic height with a period of a superlattice A. The presence of such a step structure in high-quality VSLs was proved in a number of experimental works devoted to structural research of boundaries in such VSLs. The emergence in these VSLs of such periodic system of atomic steps allows to explain the appearance of MGs in the energetic spectrum of particles in VSLs by scattering electrons on such steps. The magnitude of MGs will be well in agreement with their estimations made for this model [2,3].

In such a model VSL is approximated by the empty goffered potential channel with a periodically varying width, in which a free particle moves. The role of the crystal potential in this model is reduced only to the replacement of the free mass of a particle m_o by the effective mass m*. It is easy to see that in accordance with the basic idea [2,3] this picture is incomplete, since in such model the contribution of the crystal potential to the formation of the

superlattice effects is taken into account incompletely. The importance of such account follows from that obvious fact that besides the formation of a periodic (with a period A) atomic step system on vicinal heteroboundaries in the region of the localization of the wave function of a particle in a superlattice across a quantum well there are many internal crystallographic high-index planes with the same longitudinal translation period A, i.e. in the formation of the superlattice spectrum all these planes should make a contribution.

It is obvious that this contribution should be essential, if in the area of the steps on the quantum well boundaries there are tails of the cross wave function of a particle, whereas on the area of internal crystallographic planes the basic part of the wave function of a particle is necessary. According to what has been said, the importance of the role of the crystal potential in the formation of both the magnitude of the superlattice MGs and all physical properties of such systems is obvious. It is also important to note that if in the process of the preparation of such vicinal superlattice the system of periodic steps on boundaries for any reason or completely is expressed, or is not formed at all, internal high-index crystallographic planes exist and are in this case the unique reason of the formation of a superlattice spectrum. In the model of an empty goffered channel the disappearrance of the steps (i.e.goffered) results in the disappearance of superlattice effects. It is also necessary to emphasize that, since the crystal potential makes a contribution to the formation of the magnitude of the superlattice MGs, there is an opportunity to determine some parameters of the crystal potential from the experimentally measured magnitude of the MGs.

According to what has been said this fully applies to the VSL in quantum wires. If such VSL is created with the help of a gate, the movement of carriers in cross directions of the wire is limited, on the one side, by the semiconductor low-index surface, and on three others by the potential walls of the channel formed by an electrical field of the gate. In this case the goffering of the channel is practically absent and the crystal potential in the area of the

localization of the wave function of a particle in VSL is the principal reason of MGs formation in such structure.

Let us note that in the effective mass approximation (EMA) it is impossible to receive the superlattice spectrum of a particle in VSL initiated by the periodic structure of internal crystallographic planes, since in this approximation in the smooth (without accounting for the goffering of the walls) channel the free particle moves with effective mass m*. Therefore it is obvious that the direct accounting of the crystal potential in the MGs formation requires the exit beyond the framework of EMA. As an illustration of what has been said we shall make an estimation of the magnitude of the lower MG arising in VSL in quantum wires.

Let us present the calculation scheme. Let us consider the single-valley semiconductor of the GaAs type with a minimum of the conductivity band at the quasimomentum $\boldsymbol{k} = 0$ and the appropriate Bloch function equal in this case simply to the Bloch factor $u_0(\boldsymbol{r})$. Let us presume that we know the EMA eigenvalues $E_{n,m,\boldsymbol{k}}$ and the envelope wave functions of a particle (bending around) $F_{n,m,\boldsymbol{k}}(\boldsymbol{r})$ in a conductivity band for the channel with smooth, ungoffered walls (n and m - quantum numbers of the quantum confinement subbands correspond to the quantization along the two axes, $\boldsymbol{k}$ is the quasimomentum on wire's axis, $\boldsymbol{r}$ is the coordinate of a particle). Then the complete wave function of the particle has a kind of the product $F_{n,m,\boldsymbol{k}}(\boldsymbol{r})\, u_0(\boldsymbol{r})$. It is convenient for the realization of the minigaps estimation to use the following procedure [12]. Let us introduce further a certain (unknown) effective potential $V_{eff}(\boldsymbol{r})$, such that the complete wave functions of a particle in the EMA would be the exact solution of the Schrodinger equation with potential $V_{eff}(\boldsymbol{r})$. In this case it is natural to choose a difference $[V(\boldsymbol{r}) + U(\boldsymbol{r}) - V_{eff}(\boldsymbol{r})]$ as the operator of the perturbation which brings us beyond the limits of the EMA. Here $V(\boldsymbol{r})$ is the periodic potential of the crystal lattice, $U(\boldsymbol{r})$ - potential locating a particle in a crystal. As a result of the effect of this operator on the function $F_{n,m,\boldsymbol{k}}(\boldsymbol{r})\, u_0(\boldsymbol{r})$ we have:

$$[V(\boldsymbol{r}) + U(\boldsymbol{r}) - V_{eff}(\boldsymbol{r})] \,|\, F_{n,m,\boldsymbol{k}}(\boldsymbol{r})\, u_0(\boldsymbol{r})> = \hbar^2/2m^*[(1- m^*/m_0)\, u_0(\boldsymbol{r})\Delta F_{n,m,\boldsymbol{k}}(\boldsymbol{r}) - 2m^*/m_0 \nabla F_{n,m,\boldsymbol{k}}(\boldsymbol{r}) \nabla u_0(\boldsymbol{r})] \quad (1)$$

Further it is convenient in the rectangular coordinate system (X,Y,Z) connected with the main GaAs crystallographic axes to expand $u_0(\mathbf{r})$ in Fourier series on the vectors of a reciprocal lattice:

$$u_0(r) = \sum_{g_1 g_2 g_3} C_{g_1 g_2 g_3} e^{\frac{2\pi i}{a_0}(g_1 x + g_2 y + g_3 z)} \qquad (g_1, g_2, g_3 \text{ - integers}) \quad (2)$$

Further, we pass to the new coordinate system (X',Y', Z') which rotates around the Z axis on the angle α. Then we transform the expressions (1) and (2) into this coordinate system. Then for the convenience we cut the prime at the coordinates. In this system we will obtain new reciprocal vectors which are linear combinations of the initial vectors. These new reciprocal vectors will determine in the $\boldsymbol{k}$ - space the positions of new boundaries of the Brillouin zone, i.e. the positions of the arising minigaps. For the GaAs lattice a new basic translation period along the wire is $A = a_0/2\sin\alpha$.. We shall be limited to the simple model assuming that the one-dimensional quantum channel has a rectangular cross-section $L'_z \times L'_x$, where L'_z and L'_x are linear sizes of the channel on axes Z' and X', respectively. The axis Y' is directed along the axis of the channel. Let us also assume that the walls goffering of the channel is absent, i.e. the unique reason of the appearence of the MGs in such model can be only the crystal potential. The resultant expression for the magnitudes of lower minigaps at m, n = 1 arising from the new boundaries of the first Brillouin zone at the $k_y = \pm 2\pi \sin\alpha / a_0$ and small angles α are:

$$\Delta_{n=1,m=1}(k_y = \pm\frac{2\pi}{a_0}\sin\alpha) \approx \frac{2\pi^2\hbar^2}{m^* L_x^2}\left|C^*_{2,0,0}C_{0,0,0}\right| \frac{\sin(2\pi\frac{L_x}{a_0}\cos\alpha)}{2\pi\frac{L_x}{a_0}\cos\alpha(\cos^2\alpha - \frac{a_0^2}{4L_x^2})}\left[\frac{2m^*}{m_0} + (1-\frac{m^*}{m_0})(\sin^2\alpha + \frac{a_0^2}{4L_x^2} + \frac{a_0^2}{4L_z^2})\right] \quad (3)$$

In this model the well known solutions $F_{n,m,\boldsymbol{k}}(\boldsymbol{r})$ for the rectangular channel with infinite potential barriers are taken. We left in (3) only the principal term from the sum total at g_i which is in the total expression for Δ. We do not present here this total expression because of its awkwardness. In addition, we underestimated the real magnitude of the MG. However, (3) demonstrates the main dependencies Δ on different parameters. The main peculiarity of the expression (3) is dependence of the magnitude of the MGs on the expansion coefficients C_g in the initial coordinate system (X,Y,Z) which are determined completely by the crystal potential and on the orientation of the channel on the crystal's surface. From (3) it follows that Δ remains the finite value at $L'_z \to \infty$ since in this case we pass to the superlattice in the two-dimensional system which is confined along the X' axis by vicinal boundaries along (Z'-Y') plane. However, $\Delta \to 0$ at $L_x \to \infty$ since in this case in the resulting two-dimensional system which is confined along Z' axis the new translation period A disappears. The passage to the limit at $\alpha \to 0$ in our model implies in fact the sorting of the sequence of the quantum wires with decreasing angles α at the constant distance BD = L on fig.1. In this situation $L_x = L \cos\alpha$ and at $\alpha = 0$, $L_x = L = Na_0$ where N is the number of primitive cells of a crystal on the distance L. Thus, as is evident from (3), $\Delta \to 0$ at $\alpha \to 0$. The estimates show that for the GaAs quantum wire of 30 Å width along the surface the magnitude of lower MG approximates several meV.

Considering various orientations of low-index surfaces for different semiconductors, we have shown that two situations are possible in one-dimensional VSL.

The quantum wire is developed on the surface of a single-valley semiconductor (the minimum of the energy is in the centre of the Brillouin zone) or when in a multi-valley semiconductor the centres of the constant energy ellipsoids are projected onto the centre of the two-dimensional Brillouin zone. In this case the experimentally determined superlattice period coincides with the crystallographic period A.

If the centres of the constant energy ellipsoids in a multi-valley semiconductor are not projected to the centre of the two-dimensional Brillouin zone, then the experimentally determined period is different from the crystallographic period A.

3. Conclusions

In this work we suggested a new method of development (a new way to create) of the VSL in the quantum wires on semiconductor low-index surfaces. We showed theoretically, too, that the consideration of the only crystal potential and of the potential locating the particle in VSL results in the appearance of MGs even without taking into account the step structure of the VSL boundaries by leaving the effective mass approximation. For the cases of the rectangular quantum wire on the low-index surface of the single-valley semiconductors of the GaAs type analytical expressions have been obtained for the magnitudes of the MGs which depend on the parameters of crystal and localizing potentials as well as at the angles that define the orientation of the quantum wire on the low-index surface. It has been shown that the magnitudes of MGs approximate several meV.

References

[1] L. Esaki and R. Tsu, *IBM J.Res.Dev.* **1970**, *14*, 61.

[2] V.A. Petrov, Abstracts of the 6th All-Union conf. on the Physics of Surface Phenomena in Semicond. USSR, Kiev, *2*, 80, **1977**.

[3] V.A. Petrov, Sov. Phys. Semicond. **1978**, *12*, 219.

[4] T. Cole, A.A. Lakhani, and P.J. Stiles, Phys. Rev. Lett. **1977**, *38*, 722.

[5] V.P. Dragunov, I.G. Neizvestnyj, and V.A. Gridchin, *Fundamentals of Nanoelectronics,* Fizmatkniga, Moscow, (in Russian) **2006**.

[6] Z.D. Kvon, B.B. Kol'tsov, I.G. Neizvestnyi,V.N. Ovsyuk, JETP Letters. **1981**, 33, 571.

[7] V.A. Volkov, V.A. Petrov, and V.B. Sandomirskii, Sov.Phys.Usp. **1980**, *23*, 375.

[8] T. Ando, A. Fowler, and F. Stern, Rev. Modern. Phys. **1982**, *54*, 437.

[9] P. M. Petroff, A. C. Gossard, and W. Wiegmann, Appl.Phys.Lett. **1984**, *45*, 620.

[10] Axel Lorke and Pierre M. Petroff, Solid-State Electronics **1994**, *37*, 559.

[11] V.A. Petrov, Sov. Tech. Phys. Lett. **1978**, *4*, 285.

[12] A.M. Stoneham, *Theory of Defects in Solids*, Clarendon Press, Oxford, ch.4. **1975**.

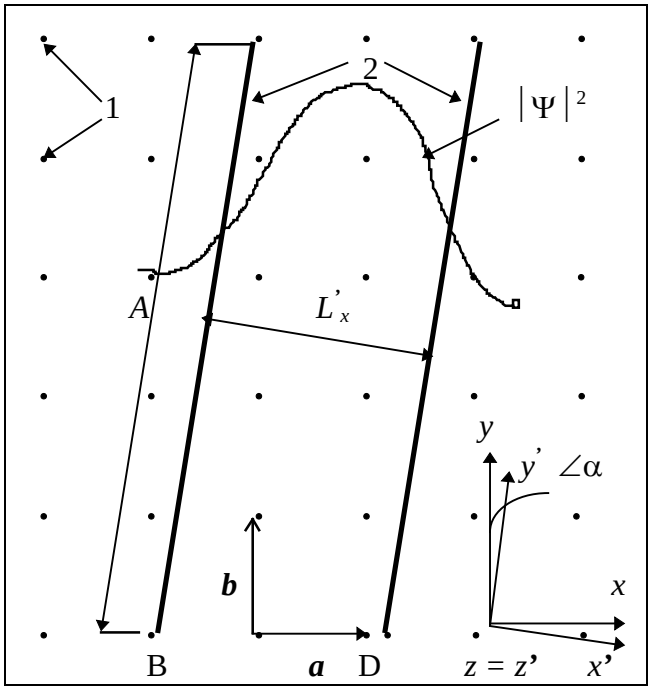

Figure 1. Vicinal quantum wire on the low-index surface; 1 - atoms in the crystal lattice; 2 - region of the particle wave function localization along the surface; **a** and **b** - basic translation vectors along the low-index surface; A-new basic translation period along the quantum wire; $\angle\alpha$ - orientation angle which determines the period A in the vicinal quantum wire; $|\Psi|^2$ - distribution of electron density on the first quantum level along the surface in the wire; (X,Y,Z) - low-index coordinate system, (X',Y',Z') - high-index coordinate system, Z = Z'.