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THE POTENTIAL DISTRIBUTION IN VERY THIN GaAs HETEROJUNCTIONS

Since the electric field at GaAs-Al_x Ga_{1-x} As interface is quite large electrons are confine within deep potential wells besides each surface. The analysis of this structure involves the self-consistent solution of the Schrödinger and Poisson equation determining the energies and the wave functions of electrons, the concentration, as well as the potential distribution depending on the temperature, surface electron densities and on the GaAs layer thickness. The results obtained were compared with the resutls obtained by the model of infinite rectangular well and by the self-consistent solution of the Schrödinger and Poisson equation.

1. INTRODUCTION. Some ten years ago the first theoretical [1] and experimental papers [2] were published relevent to the very thin layers of the GaAs-Al_x Ga_{1-x} As heterojunctions. By special technological procedure (molecular beam epitaxy)it is possible to the thickness of particular layers to be smaller than 50Å. In casses of smaller thicknesses, couplings between adjacent wells become important; the consequence is the superlattice formation [2]. However, if thicknesses $Al_xGa_{1-x}As$ layers are relatively big(biger than 250Å), all electrons confine in the GaAs layers [3,4]. Such structures were considered: (a) by the model of infinite or finite rectangular well [3,4] or (b) by the self-consistent solving the Shrödinger and Poisson equation (The Schrödinger equation was solved by the variational method, [5].) The problem of the potential determination in the MISIM structure (which reduces to the problem considered in this paper) was solved in [6] by means of the confluent hipergeometrical functions, but not self-consistently.

This paper will provide a general theoretical approach and the numerical results of the self-consistent solution for the case of GaAs layer. The numerical results will be compared with the respective results obtained by classical solving of the Poisson equation and by the model of infinite rectangular well.

2. THE THEORY AND THE NUMERICAL RESULTS. Let us observe the periodical structure presented in Fig.1. The structure can be doped in two ways [6]:

a) the entire structure is uniformly doped by donors (or

acceptors) of N_D concentration (uniform doping case) and b) only $Al_x Ga_{1-x}$ As layers are doped, while GaAs layers remain undoped (modulation doping case). In both cases a depletion of electrons occurs in $Al_x Ga_{1-x}$ As layers they concentrate in potential wells in the GaAs layers. The periodicity of the structure and the already mentioned condition ($d_1 >> d$) enables the problem to be observed only for in the region $0 \leq x \leq d$.

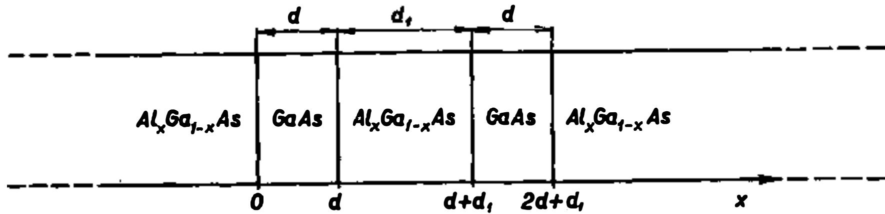

Fig.1. - The schematic diagram of the semiconductor superlattice.

Wave function $\psi_i(x)$ describing the electrons at the i-th energy level E_i is the solution of the Schrödinger equation:

$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi_i}{dx^2} - e\phi(x)\psi_i = E_i\psi_i \qquad (1)$$

where m* is the effective mass, and $e\phi(x)$ the potential electron energy. Assuming that the potential barrier for x=0 and x=d is quite high, it could be assumed that the wave function is annuled at these points.

Though the potential distribution in GaAs layer, from the theoretical and practical point of view, is symmetrical with respect to x=d/2, we shall assume, for the generalization of the opservation, an asymmetrical distribution. The surface electron densities

$$N_{S1} = \int_0^{x_o} n(x)dx \text{ and } N_{S2} = \int_{x_o}^{d} n(x)dx \qquad (2)$$

are, in the general assymetrical case different. In (2) x_o is determined from the condition:

$$\left.\frac{d\phi}{dx}\right|_{x=0} = 0 \ . \qquad (3)$$

Concentration along the layer is [7]:

$$n(x) = \frac{m^*kT}{\pi\hbar^2} \sum_i \ln(1+\exp(\frac{E_F-E_i}{kT}))\cdot\psi_i^2, \qquad (4)$$

E_F is the energy of the Fermi level and it is determined from the electrical neutrality conditions.

The Poisson equation for this case reads:

$$\frac{d^2\phi}{dx^2} = \frac{e}{\varepsilon_s}\left|n(x)-\theta\cdot N_D\right|, \quad \theta = 0 \text{ and } 1 , \qquad (5)$$

where ε_s is the dielectric constant of the semiconductor, $\theta=0$ for the modulating doping case, while $\theta=1$ in the uniform doping case.

The boundary conditions are:

$$\phi(0) = 0 \quad \text{and} \quad \left.\frac{d\phi}{dx}\right|_{x=0} = \frac{e}{\varepsilon_s}\,[N_{S1} - \theta\, N_D\, x_o]. \qquad (6)$$

The potential obtained from the classical Poisson equation (the expression for concentration n(x) is of the classical form and not of quantum form as expression (4)), was taken as the trial potential.

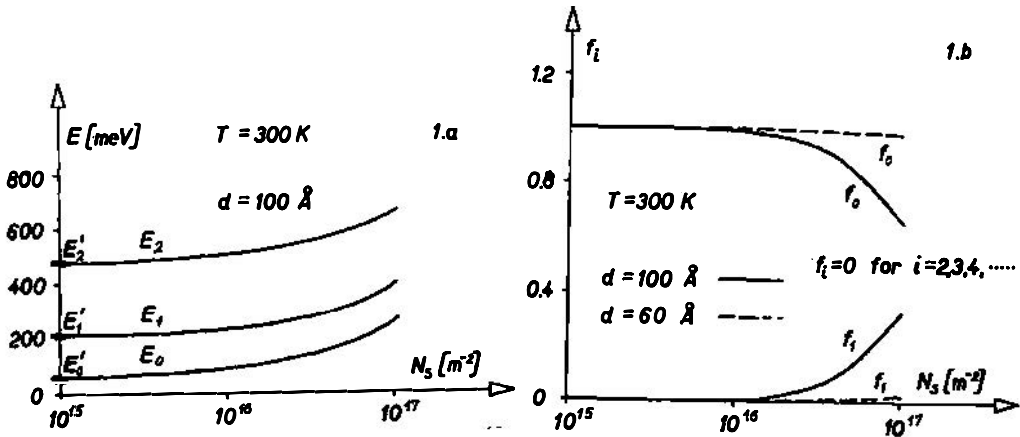

Fig.2. - a) The dependence of the first three lowest energy levels on the surface density N_S. Energies E_0', E_1' and E_2' are marked on the ordinate; they were obtained by the infinite rectangular well model.
b) The dependence of the filling factor $f_i=N_i/N_s$ on N_s.

The numerical results are supplied for symmetrical GaAs layers (x_o=d/2) of the surface densities N_S from $10^{15}m^{-2}$ to $10^{17}m^{-2}$ ($N_S=N_{S1}+N_{S2}$). The layer thicknesses were d=60Å and d=100Å, and the temperature T=300K and T=77K. The modulation doping case is considered. The numerical results were presented in Figs 2 and 3. The dependence of quantities presented in Figs 2 and 3 at T=77K differs very little from the respective quantities at T=300K, for example, E_o(77K, $3\cdot10^{16}m^{-2}$)=126,76 meV, while E_o(300K, $3\cdot10^{16}m^{-2}$)=126,22meV; that is E_1(300K, N_S) was not displayed in Fig.3.

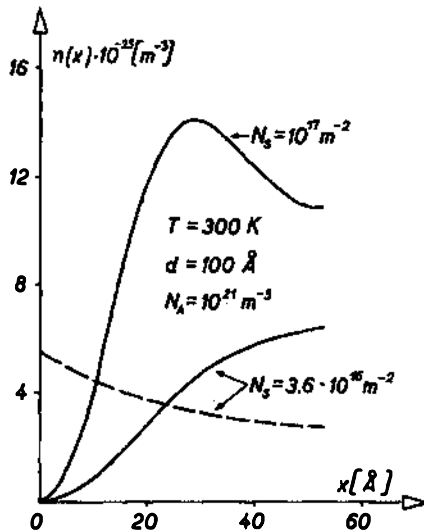

Fig.3. - The dependence of the concentration n on x; T=300K, d=100Å and $N_S=3,6\cdot10^{16}$ (the full line represents the results obtained by a selfconsistent solving; dotted line-those obtained by a classical method.

4. CONCLUSION. Assuming the thickness of the $Al_xGa_{1-x}As$ layer to be very large the paper presents the theoretical analysis and the numerical results of the self-consistent solution for the GaAs layer.

A comparison between the self-consistently obtained energy levels and the respective ones obtained by the infinite rectangular well model was made (which corresponds to the case N_s=0). From Fig.2a it is seen that the deviations are considerable, especially at higher surface densities N_s. This points out to the indispensability of the self-consistent solution, though paper [3] claims the opposite.

For thicknesses d=60Å and d=100Å (realized as in [3] the conditions of the quantum limit are, for the large ranges of values N_s, almost ideally fulfilled. For thicknesses d<100Å (from Fig. 2b) we should limit ourselves to two energy levels (even at T=300K).

From Fig.3 it is seen that the concentration dependence n(x) obtained by solving the classical Poisson equation differs essentially from the respective self-consistent solution, at all other same conditions. The differences are qualitative (only the form of the dependence) and quantitative. Besides, at higher values of N_s two maxima (symmetrical with respect to x=d/2) and a minimum (for x=d/2) appear at the dependence n(x) which is the consequence of the fact that at lower N_s the second energy level is partially occupied (Fig. 2b). Therefore it is obvious that the quantum treatmens is indispensably because one does not yield even the roughest qualitative agreement.

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