Extended Abstracts of the 16th (1984 International) Conference on Solid State Devices and Materials, Kobe, 1984, pp. 599-602

Self-Consistent Calculations of Two-Dimensional Electron Density in $GaAs/Al_xGa_{1-x}As$ Heterostructures

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Sheet density of the two-dimensional electron gas in modulation doped GaAs/$Al_xGa_{1-x}As$ heterostructures have been calculated self-consistently as functions of the doping density in n-$Al_xGa_{1-x}As$ and the thickness of the un-doped $Al_xGa_{1-x}As$ layer for x = 0.17 to 0.33 and lattice temperatures at 4.2 and 77K. It is found that the triangular approximation and other treatments reported so far will not give a good result. Present results indicate that the penetration of the electron functions into the un-doped $Al_xGa_{1-x}As$ layer plays an important role in determining the device parameters.

§1. Introduction

Recently, several kinds of GaAs/$Al_xGa_{1-x}As$ field effect transistors have been proposed[1,2,3], which are fabricated with molecular beam epitaxy tequniques. HEMT is the most famous among them, in which high switching speed and high electron mobility at low temperatures are achieved.

In view of design of modulation doped GaAs/$Al_xGa_{1-x}As$ field effect transistors, it is important to know the properties of hetero-interface as a function of doping concentrations in n type $Al_xGa_{1-x}As$ layer. In order to analyse these properties, several methods, for example, the triangular potential approximation or variational treatment[4], have been reported so far. Such methods, however, are not sufficient to provide a satisfactory result because they neglect the penetration of the electron wave functions into the $Al_xGa_{1-x}As$ layer. In other words, the assumption of the infinite discontinuity of the conduction band edge at the hetero-interface is not correct in this GaAs/$Al_xGa_{1-x}As$ system.

We propose more refined analysis which utilize self-consistent calculations by taking into account the finite discontinuity of the conduction bands at the interface. The method has been successfully applied to the case of Si inversion layer to investigate electronic properties[5] and also adopted to study the two-dimensional system in GaAs/$Al_xGa_{1-x}As$ heterojunctions[6]. The electron density of the two-dimensional electron gas (2DEG) in modulation doped GaAs/$Al_xGa_{1-x}As$ heterostructure have been calculated self-consistently as a function of the un-doped $Al_xGa_{1-x}As$ for x = 0.17 to 0.33 and lattice temperatures at 4.2 and 77K. The calculations were carried out by solving Schrodinger equation and Poisson equation self-consistently. The result show that the penetration of the electron wave functions into the un-doped $Al_xGa_{1-x}As$ layer plays an important role in device parameters.

§2. Self-consistent calculations

Shown in Fig.1 is the schematic diagram of a GaAs/$Al_xGa_{1-x}As$ heterostructure dealt with in the present paper.

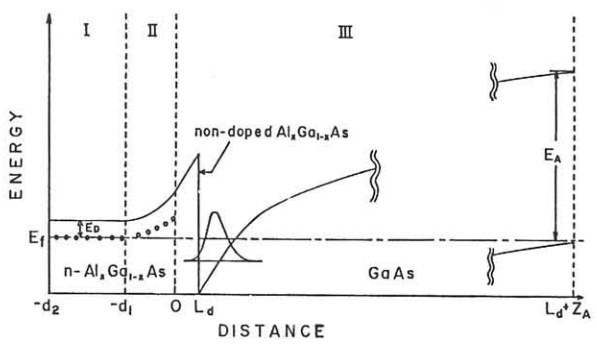

Fig. 1 Schmatic sketch of the model of $Al_xGa_{1-x}As$ single hetero structure.

We assume that this system is devided into three regions which are denoted by I, II, III. Region III denotes spacer-layer (non doped $Al_xGa_{1-x}As$) and GaAs layer which is undoped. $Al_xGa_{1-x}As$ layer in the region II is fully depleted and, thus, all of the donor are ionized to supply the electrons in the heterointerface resulting in forming 2DEG. The conduction band edge, subband energies and Fermi energy are measured from the conduction band edge minimum. We have to note that the depletion approximation will introduce an error in evaluating the charge density in the region II, especially in the case of high donor densities. More refined analysis in this region by Lee et al.[7], where they used Fermi-Dirac statistics for the electrons captured by the donors and Ehrenberg relation for the Fermi integral. In the present work we used this refined method to solve Poisson equation in this region and found that the results give a good agreement with the depletion approximation for higher donor densities as shown later. In this paper, therefore, we report the results calculated by the depletion approximation and more refined analysis will be reported elsewhere[8].

Now we calculate the conduction band edge $\phi_I(z)$ in the region I by solving Poisson equation given by

$$\frac{d^2\phi_I}{dz^2} = 0 \tag{1}$$

where ϕ_I is the conduction edge potential measured from the conduction band edge minimum at the interface. Therefore conduction band edge in the region I is given by

$$-e\phi_I(z) = E_f + E_D \tag{2}$$

where E_f is the Fermi energy and E_D is the activation energy of n-$Al_xGa_{1-x}As$.

Conduction band edge potential $\phi_{II}(z)$ in the region II is given by

$$\frac{d^2\phi_{II}}{dz^2} = -\frac{e \times N_D}{\varepsilon} \tag{3}$$

where N_D is the net donor density in n-$Al_xGa_{1-x}As$ layer and ε is the dielectric constant of n-$Al_xGa_{1-x}As$. The boundary condition is given by

$$\left.\frac{d\phi_{II}}{dz}\right|_{z=-d_1} = 0 \tag{4}$$

$$-e\phi_{II}(-d_1) = E_f + E_D \tag{5}$$

Therefore, conduction band edge $\phi_{II}(z)$ and its first derivative are given by

$$\phi_{II}(z) = \frac{eN_D}{2}(z + d_1)^2 + E_f + E_D \tag{6}$$

$$\frac{d\phi_{II}}{dz} = \frac{eN_D}{\varepsilon}(z + d_1) \tag{7}$$

In order to solve equilibrium state in area III, we have to solve effective mass equation and Poisson equation self-consistently. The envelope function $\zeta_i(z)$ satisfies

$$\left[-\frac{\hbar^2}{2m_z}\frac{\partial^2}{\partial z^2} + \phi_{III}(z)\right]\zeta_i(z) = E_i'\,\zeta_i(z) \tag{8}$$

where m_z is the effective mass perpendicular to the hetero interface. E_i' is given by

$$E_i' = E_i - \frac{\hbar^2}{2m_\perp}(k_x^2 + k_y^2) \tag{9}$$

where $m_\perp$ is the effective mass parallel to the interface.

The potential $\phi_{III}(z)$ is written as

$$\phi_{III}(z) = \phi_o\Theta(z) + \phi_H(z) + \phi_{xc}(z) \tag{10}$$

where ϕ_o and $\Theta(z)$ are the magnitude of the discontinuity of the conduction band edge at the interface and the step function, respectively. The Hartree potential $\phi_H(z)$ is given by

$$\frac{d^2\phi_{III}}{dz^2} = -\frac{e[\Sigma_i N_i|\zeta_i(z)|^2 + N_A(z)]}{\varepsilon} \tag{11}$$

where N_i (z) and $N_A(z)$ are the subband electron density and the net accepter density in GaAs layer, respectively. Surface electron sheet density

N_s is obtained from charge neutrality as follows.

$$N_s = N_D Z_D - N_A Z_A \tag{12}$$

where Z_D is the depletion width of n-$Al_xGa_{1-x}As$ layer. Z_A is the width of GaAs layer which is given by

$$Z_A = \sqrt{\frac{2\varepsilon E_g}{e N_A}} \tag{13}$$

where E_g is the band gap of GaAs layer. And we assumed that the accepter binding energy E_A in GaAs layer as illustrated in Fig. 2 is much smaller than the band gap. The energy gap of GaAs is given by

$$E_g(T) = E_o - \frac{\alpha T^2}{T + \beta} \tag{14}$$

where E_o, α and β are 1.519(eV), 5.405×10^{-4} (eV/K) and 204(K), respectively[9].

Assuming the potential and its first derivative are continuous at z = 0, we get N_D and Z_D from above equations as follows.

$$Z_D = d_1 = \frac{2\phi(0)}{\left.\frac{d\phi}{dz}\right|_{z=0}} \tag{16}$$

$$N_D = \frac{\varepsilon\left(\left.\frac{d\phi}{dz}\right|_{z=0}\right)^2}{2e\phi(0)} \tag{15}$$

§3. Results and discussion

Since the ionization energy of the donors in n-$Al_xGa_{1-x}As$ is not known well, we assumed three different values, 50, 100, and 150meV for the present calculations. In this abstract we show the self-consistent results on the heterostructures with 60Å un-doped $Al_xGa_{1-x}As$ layer, 100meV donor ionization energy, and x = 0.17 to 0.33 at T = 4.2K, where the conduction band discontinuity is assumed to be given by x in eV.

Figure 2 shows the electron densities in GaAs as a function of the donor density in n-$Al_xGa_{1-x}As$ for x = 0.33, 0.30, 0,25 and 0.17. We find in Fig. 2 that the interface electron density increases with increasing the donor concentrations in n-$Al_xGa_{1-x}As$ and with increasing the aluminium contents x. Such a behavior is similar to the result obtained from other methods but the absolute values are not in good agreement due to the fact stated above.

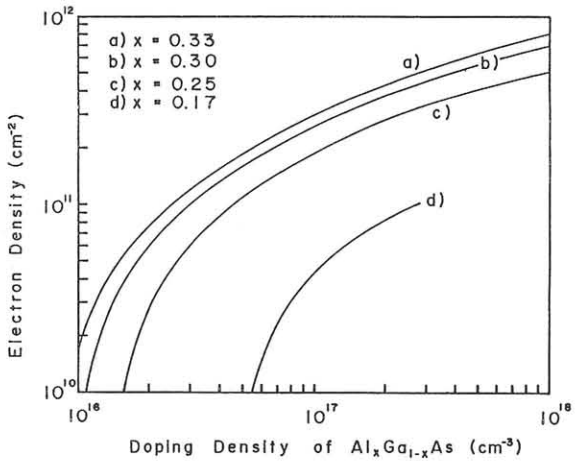

Fig. 2 Electron density in GaAs vs. donor density in n-$Al_xGa_{1-x}As$ with 60Å spacer at T = 4.2K.

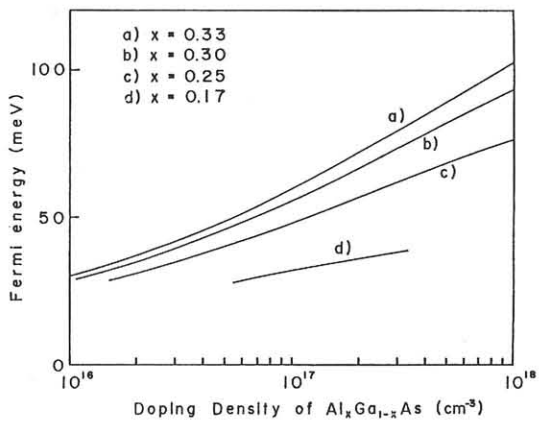

Fig. 3 Self-consistent results of Fermi energy vs. doping density of $Al_xGa_{1-x}As$ with the aluminium content x as a parameter.

We present Fermi energies for the interface electrons as a function of doping density in n-$Al_xGa_{1-x}As$. Fermi energy increases with increasing the doping density due to the increase in the electron density, where the Fermi energy is measured from the conduction band edge of GaAs at the interface. It is found that the electrons are not

confined in the interface for a smaller value of aluminium content x and for a large value of doping density in n-$Al_xGa_{1-x}As$. Therefore we excluded such regions in Fig. 3.

Figure 4 shows the calculated depletion width of n-$Al_xGa_{1-x}As$ as a function of the doping density. Since the interface electrons are supplied from the donors in the n-$Al_xGa_{1-x}As$, the depletion width decreases with increasing the doping density.

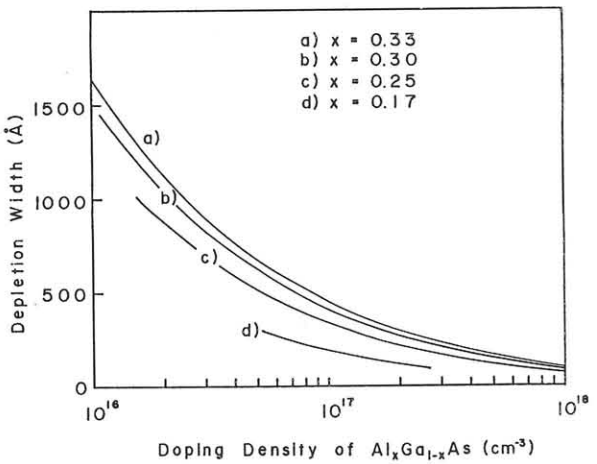

Fig. 4 Self-consistent results of the depletion width vs. doping density of $Al_xGa_{1-x}As$ with the aluminium content x as a parameter.

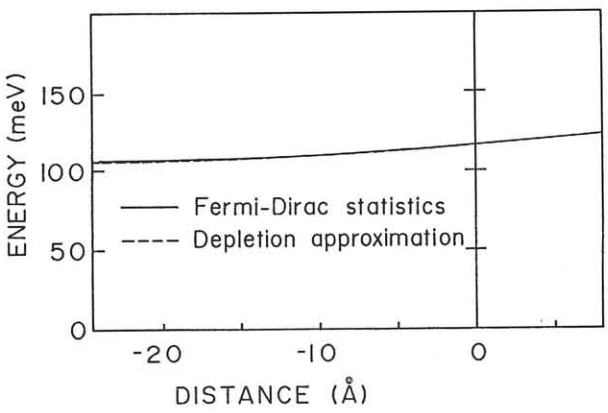

Fig. 5 The conduction band edge level in n-$Al_xGa_{1-x}As$ layer for $N_s = 10^{12}cm^{-2}$. Solid line: Fermi-Dirac statistics; Dotted line: Depletion approximation.

As pointed out earlier, the depletion approximation is expected not to give a satisfactory result in the region II. We, therefore, solved Poisson equation, using eq.(6) of reference 8, and the resulting curve of conduction band edge in the regions II and III are shown by solid curve in Fig. 5 for $N = 1.0\times10^{12}cm^{-2}$, where the result of the depletion approximation is also plotted by dashed curve. As seen in Fig. 5, we find no noticeable difference between the two approximation methods. However, it was found that the results for smaller values of N_s do not agree well[8].

In conclusion we present self-consistent calculations of the 2DEG density as a donor density in n-$Al_xGa_{1-x}As$. The present results give a very important information about the doping density and the width of the n-$Al_xGa_{1-x}As$ required to get a desired electron density in the GaAs layer and thus a design principle of the HEMT.

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