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ELECTRONIC PROPERTIES OF A HEAVILY-DOPED n-TYPE GaAs–$Ga_{1-x}Al_xAs$ SUPERLATTICE

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The subband structure of a heavily-doped n-type GaAs–$Ga_{1-x}Al_xAs$ superlattice is calculated self-consistently. The band bending becomes crucial in the case of modulation doping especially at high electron concentrations. Results are in good agreement with recent experiments. Low-temperature mobilities parallel to the layers are also calculated as a function of electron concentrations.

1. Introduction

The evolution of molecular beam epitaxy has allowed access to man-made semiconductor superlattices, which consist of periodic alternate thin layers of two semiconductors. Heterostructures made of GaAs and $Ga_{1-x}Al_xAs$ have extensively been studied both experimentally and theoretically [1–4]. From various experimental investigations, it has been known that the boundary is sharp to within a lattice constant and that a simple model of a sequent square-well potential works quite well.

Recently Dingle et al. applied a modulation doping technique [5,6]. In this technique only the $Ga_{1-x}Al_xAs$ layers are doped and the GaAs layers are not. Donors in the $Ga_{1-x}Al_xAs$ layers are ionized and the electrons are transferred to the GaAs layers. Measured mobilities parallel to the layers are much larger than those of a uniformly-doped GaAs–$Ga_{1-x}Al_xAs$, and are even larger than in bulk spatial separation between carriers and scatterers. However a detailed understanding of the mobility has not been achieved yet. In this paper we calculate the mobilities of electrons parallel to the layers both in the modulation doping case and in the uniform doping case. In such heavily-doped cases we should also consider effects of doping on the subband structure. A band bending effect caused by charge transfer is calculated self-consistently in the Hartree approximation.

In section 2 calculated results of the subband structure are presented and compared with experiments. In section 3 mobilities are calculated and compared with experiments.

2. Subband structure

We calculate the subband structure on the base of effective mass approximation. The motion of electrons parallel to the layers can be described by a free electron state with certain effective mass m. As for the motion perpendicular to the layers we should consider a potential caused by a superlattice. In the calculation we use a sequent square well potential, where the $Ga_{1-x}Al_xAs$ layer is replaced by a potential barrier with a height V_0. All the donors are assumed to be ionized and are replaced by a uniform positive charge distribution. Further the potential arising from the electrons themselves is included self-consistently in the Hartree approximation. In order to solve the Schrödinger equation in this direction we expand the periodic part of the wavefunction and the potential in terms of Fourier series. Then the problem is reduced to solving the infinite simultaneous equations of the Fourier

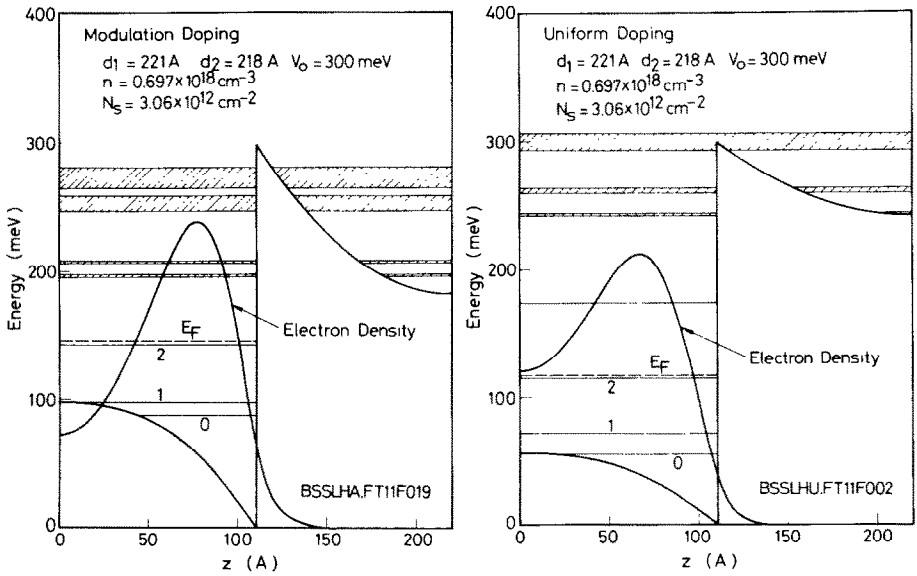

Fig. 1. Calculated energy levels, density distribution of electrons, and the self-consistent potential in the case of modulation doping. The subband widths are described by hatches.

Fig. 2. Calculated energy levels, density distribution of electrons, and the self-consistent potential in the case of uniform doping. The parameters are same as in the fig. 1.

components. In the actual calculation we truncate the infinite series at certain component which gives a convergent result.

We use $m = 0.068\ m_0$ and a static dielectric constant $\kappa = 12.9$ in the calculation considered below. Fig. 1 shows a calculated result of the density distribution, potential energies and energy spectra in the modulation doping case. Here we choose the z axis in the superlattice direction and the xy plane at the center of the GaAs layer. d_1 and d_2 are the thickness of the GaAl layer and the $Ga_{1-x}Al_xAs$ layer, respectively. N_S and n are the electron concentration in a unit area and a unit volume, respectively, with the relation $N_S = nd$, where d is defined by $d = d_1 + d_2$. Couplings between adjacent layers are weak for electrons in the three lowest subbands. The increase and decrease of the potential energy at $z = 0$ and $z = d/2$, respectively, are very large, and electrons are pushed toward the interface strongly if we include the band bending. Consequently, the lowest and next lowest subbands are already close to two accumulation layer wavefunctions, which are coupled into bonding and antibonding levels.

Fig. 2 shows a calculated result in the uniform doping case, which corresponds to the fig. 1. The band bending effect is not so important as in the case of modulation doping, but it is sufficiently appreciable in comparison with the case of a square well potential.

Fig. 3 shows calculated energy spectra of the modulation doping case as a function of the electron concentration. The Fermi energy, E_F, and the potential energies at $z = 0$ and $z = d/2$ are also included. The Fermi level touches the bottom of the first excited subband around $N_S \sim 0.8 \times 10^{12}$ cm^{-2} and that of the second excited subband around $N_S \sim 3.3 \times 10^{12}$ cm^{-2}. Because of the band bending the energy of levels bounded in the GaAs layer increases with N_S, and the bottom of the ground subband is especially influenced and approaches to the bottom of the first excited subband. Around the electron concentration where they cross the line corresponding to the potential at $z = d/2$, widths of the subband increase and their characters turn into three-dimensional. Above $N_S \sim 4 \times 10^{12}$ cm^{-2} the electron density distribution becomes extended as begins to have a considerable amount in the $Ga_{1-x}Al_xAs$ layer.

Many-body effects such as exchange and correlation are also studied in the density-functional formulation. However they are not so important as in inversion and accumulation layers on Si [7]. This is because the effective mass of electrons is much smaller than in Si and the effective electron concentration is sufficiently large in GaAs.

Optical absorption spectra have also been studied by means of calculating dynamical conductivity. The local field effect becomes important when the wavefunction is localized in the GaAs layers, and makes resonance positions shift to higher energy side considerably.

Störmer et al. measured the Shubnikov–De Haas oscillation of the conductivity along the xy plane in samples corresponding to the fig. 1. They observed two periods which are very close to each other, and obtained the energy separation of

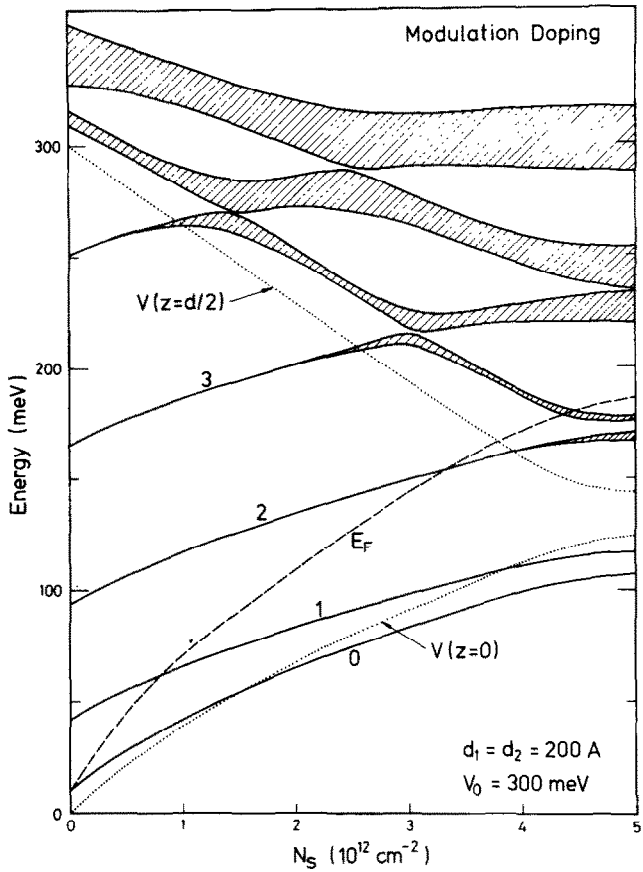

Fig. 3. Calculated energy spectra as a function of the electron concentration in the modulation doping case. The Fermi energy and the potential energy at $z = 0$ and $z = d/2$ are also shown. The subband widths are described by hatches.

the lowest two subbands as 8.6 meV [5,6]. The present calculation gives 9.4 meV in excellent agreement with their experiments. We should notice that it is given by 26.7 meV if we neglect the band bending effect. Thus we can conclude that the self-consistent determination of the band bending is crucial in this system.

3. Mobility

Low-temperature mobilities parallel to the layers are calculated with the parameters: $d_1 = d_2 = 200$ Å and $V_0 = 300$ meV. Assumed scattering mechanisms are the Coulomb scattering from donor ions and surface roughness scattering at the inter-

face. The scattering matrix elements are calculated in the lowest Born approximation, and a screening effect is included in the random phase approximation. All the donors are assumed to be ionized and to have a uniform distribution in the $Ga_{1-x}Al_xAs$ layers for the modulation doping case, and in all the layers for the uniform doping case. As for the interface roughness potential we adopt a simple model which has already been used and successful in the inversion layer of a Si-MOS [8]. We have treated the lowest two subbands by appropriate variational wavefunctions including band bending effects. Electrons are regarded as bounded in each GaAs layer and interaction between different layers are neglected. The mobilities are calculated by solving coupled Boltzmann equations and intersubband scattering effects are included when the higher subband is occupied [9,10].

Fig. 4 shows the calculated mobilities limited by the Coulomb scattering from donor ions as a function of the carrier concentration in a unit area. Results in both modulation doping and uniform doping cases are shown. The dashed lines represent mobilities which do not include band bending effects. The dotted lines represent those in the case that occupation of excited subbands is completely neglected. Decrease of mobilities from the dotted lines to the dashed lines arises from intersubband scattering when electrons occupy the first excited subband. A discontinuous drop reflects the step-function density of states in the two-dimensional system. The dashed lines are reduced to the solid lines when the band bending effects are included. As seen in the figure the band bending effect is apprecianle in the modulation doping at high carrier concentrations. The mobility decreases because electrons

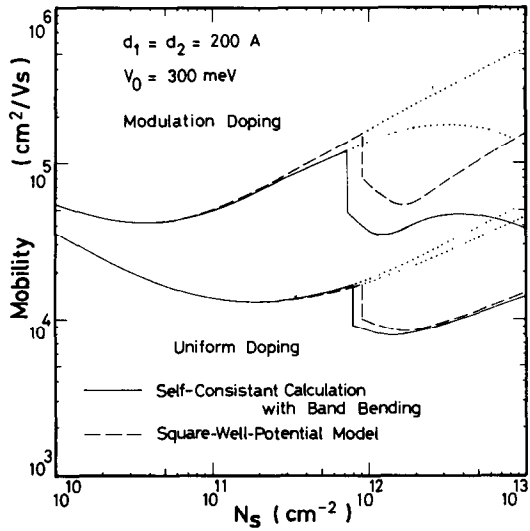

Fig. 4. Calculated Hall mobilities limited by the Coulomb scattering from donor ions as a function of electron concentration.

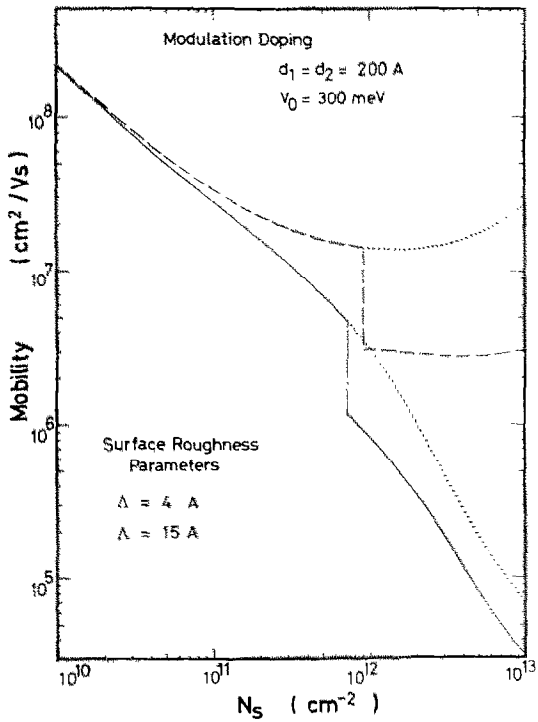

Fig. 5. Calculated Hall mobilities limited by interface roughness scattering in the modulation doping case.

are pushed toward the interface and scattering strength increases.

Fig. 5 shows the calculated mobilities limited by interface roughness scattering in the modulation doping case. In the figure Δ is the mean-square deviation of the height and Λ is the lateral spatial decay rate of interface roughness. We have assumed irregularities similar to those assumed at Si–SiO_2 interface [10,11]. The notation in the figure is exactly the same as in fig. 4. The dashed line is reduced to the solid line when the band bending effect is included. Mobilities are reduced considerably since electrons are pushed toward the rough interface. Absolute values of the mobility are much larger than those of the mobility limited by the Coulomb scattering, and the interface roughness is not important in this system.

The present calculation has shown that the mobility limited by Coulomb scattering in the modulation doping case is about one order of magnitude larger than that in the uniform doping case for $N_S \gg 10^{11}$ cm^{-2}. This agrees with the experimental observation of Dingle et al, qualitatively, but the calculated absolute values seem to be much larger than the observed ones [5,6]. For the modulation doping case the observed Hall mobility μ_H is about 1.6×10^4 $cm^2/V \cdot S$ at $N_S \sim 1.5 \times 10^{11}$ cm^{-2} after Dingle et al., while the calculated μ_H is 5.8×10^4 $cm^2/V \cdot S$. For the uniform

doping case the observed one is typically $\mu_H \sim 1 \times 10^3$ cm^2/V · S at $N_S \sim 3 \times 10^{11}$ cm^{-2}, while the calculated μ_H is 1.3×10^4 cm^2/V · S. The disagreement is left for future study.

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