Sample Parameters of Degenerate Semiconductor Superlattices

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The Shubnikov–de Haas oscillations of InP with a periodical planar doping with Si were studied at 4.2K in fields of 0–14T. By confronting the oscillation frequencies detected experimentally with the ones predicted on the basis of the effective mass approximation the carrier population of the superlattice minibands and the characteristic width of the doped layer were obtained. The width of the doped layer obtained in this way is in good agreement with the value obtained from CV profiling measurements on the same structures.

I. Introduction

Semiconductors in which the dopant atoms are confined to a single or a few monolayers of the semiconductor lattice are of much technological importance due to their applications in novel semiconductor devices[1]. In an ideal $\delta-$doped superlattice (SL) a monolayer of donor impurities is introduced periodically into the host crystal during the epitaxial growth process. The characteristic parameters of a $\delta-$doped superlattice sample are the density of donor atoms in the doping layers, n_D and the period of the doping profile, d. In real samples, thermal diffusion of the donors atoms into the host crystal may occur; in this case the distribution of donor atoms along the growth direction can be approximated by a Gaussian function with a full width at half maximum Δ[1]. The non-zero thickness of the donor layer is reflected upon the energy spectrum and miniband filling of the superlattice[2]. In addition, the presence of background ionized impurities also has influence on the electronic structure, however, these impurities can be neutralized by illuminating the sample at low temperatures; after illumination the areal density of free carriers per superlattice period can be taken as a good approximation to be equal to the density of donors, i.e. $n_S = n_D$ [3].

The characteristic parameters of a given $\delta-$doped SL sample determine to a great extent its optical and electrical properties. For instance in GaAs, with an areal carrier density fixed at about $1.2 \times 10^{12}\mathrm{cm}^2$, when the doping period is decreased from 500 to 100Å the photoluminescence spectrum associated with the presence of the $\delta-$layers changes from a narrow emission band with a cut–off energy near the band-edge to a broad emission band with a cut–off energy about 60 meV above the renormalized GaAs bandgap[4] (see also [5]). Similarly, for a fixed doping level the absorption threshold is pushed upwards when the superlattice period is made shorter[6]. These observations are in good agreement with the theoretical calculations, made in the effective mass approximation and using the characteristic sample parameters as input[7]. Shubnikov–de Haas experiments in tilted fields demonstrate the effect of coupling between adjacent $\delta-$wells upon the shape of the Fermi surface[8]; the extremal cross-section areas of the Fermi surface and their dependence on the angle between the magnetic field and the SL axis are

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also well reproduced by the same theoretical model[9]. Thus, parameters d, n_S and Δ form the basis for the modelling of the electronic structure of a $\delta-$doped superlattice, and their knowledge is a pre-requisite for the understanding of the optical and electronic properties of a given sample.

The period of the $\delta-$doped superlattice can be established accurately during the growth process; the remaining parameters (the carrier density n_S and the spreading of the donor atoms Δ) are more difficult to control during the growth, and should be established independently. For a sample with an isolated $\delta-$well (or equivalently a SL of period large enough to uncouple the $\delta-$wells), it has been demonstrated that both n_S and Δ can be determined simultaneously from the sample's transverse Shubnikov-de Haas spectrum[10]. The procedure is based upon the linear dependence between the carrier population in a given subband and a frequency of oscillation in the magnetoresistance of the sample. For a superlattice, however, the energy dispersion for movement across the layers implies that the relation between the population of a given miniband and the corresponding oscillatory magnetoresistance frequency must be calculated self-consistently[9]. To avoid this, several authors have approximated the density of states for each miniband by either a strictly two–dimensional or a three–dimensional form[5,11]; the sample parameters obtained in this way, however, are only approximate.

In this paper, we present results obtained on $\delta-$doped InP superlattices obtained by Shubnikov–de Haas and capacitance-voltage (CV) measurements. By comparing the measured frequencies of oscillation in the magnetoresistance to the values predicted by the self-consistent calculations, the best fit values of n_S and Δ are determined. The width of the donor layers, Δ, obtained from the analysis of the Shubnikov–de Haas (SdH) spectra, is in good agreement with the width of the donor layer which is extracted from the capacitance–voltage profiling for the same samples.

II. Numerical procedure

The electronic structure calculations for the $\delta-$doped superlattice were performed in the effective mass approximation by solving self–consistently the Schrödinger and Poisson equations: details of the theoretical model and a description of the sequence of steps taken in the self-consistent procedure are described in Ref. [7]. Throughout this paper atomic units are used, whereby the units of length, energy and mass are $a_B = \frac{\epsilon\hbar^2}{m^* e^2}$, $\hbar^2/m^* a_B^2$, and m^*, respectively; in this unit system the unit of magnetic field is $B_0 = \frac{\hbar}{a_B^2 e}$. The distribution of ionized donors can be approximated by a Gaussian function[1]

$$N_D(z) = n_D \sqrt{\frac{4\ln 2}{\pi\Delta^2}} \exp\left[-4\ln 2\left(\frac{z}{\Delta}\right)^2\right]$$

where Δ is the FWHM and is related to the diffusion coefficient D according to $\Delta = 4\sqrt{D\tau\ln 2}$, where τ is the diffusion time. As the starting potential for the self-consistent iterations we used the Thomas-Fermi approximation for a single $\delta-$well, as given by Ioriatti[1] [12]:

$$V(z) = -\frac{1}{2}\frac{\alpha^2}{(\alpha|z| + z_0)^4} \qquad (1)$$

where $\alpha = 2/15\pi$ and $z_0 = \left(\alpha^3\pi n_S\right)^{1/5}$.

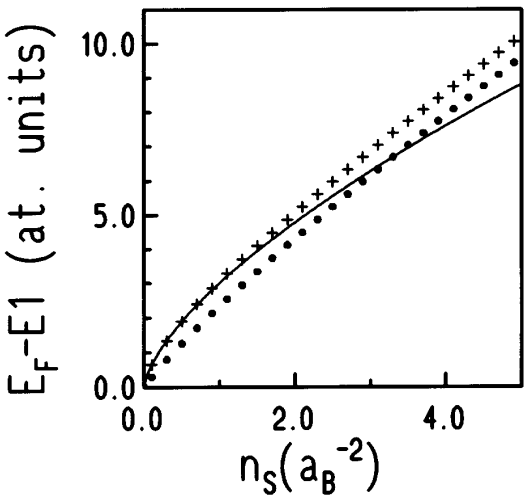

Figure 1. Calculated Fermi energy for a SL with parameters $d = 2a_B$ as a function of n_S (crosses). Full line is the limiting 3D approximation. Full circles correspond to the 2D Thomas-Fermi approximation, obtained from a numerical solution for the potential given by Eq.(1).

[1] The factor $\frac{1}{2}$ arises here because of the system of units used.

Fig. 1 shows the calculated dependence of the Fermi energy on the areal density n_S for a SL of period $d = 2a_B$ and $\Delta = 0.2a_B$ (full circles). Also shown in Fig. 1 is the Fermi energy dependence on n_S for a free electron gas, $E_F^{3D} = \frac{1}{2}(3\pi^2 n_S/d)^{2/3}$ (full line), and the dependence of the Fermi energy on n_S in the two-dimensional Thomas-Fermi approximation (full circles), obtained from a numerical solution to the Schrödinger equation with the confining potential given by Eq.(1). At low values of n_S, the wells are shallow and the coupling between neighboring wells is strong, so that E_F follows the bulk dependence E_F^{3D}. At high concentrations the coupling between adjacent wells decreases, and the dependence of E_F on n_S approaches the same linear dependence as the Thomas-Fermi approximation for an isolated $\delta-$well. The 2D behavior at large n_S illustrates the point that at very high doping levels the $\delta-$wells are uncoupled even for very short period SL's, as previewed from *ab-initio* calculations[13].

The connection between the output of the numerical calculations and the results of the transverse Shubnikov-de Haas measurements (when the magnetic field is applied parallel to the axis of the superlattice) is based upon the fact that if plotted against inverse field the magnetoresistance oscillations of a $\delta-$doped superlattice display a set of frequencies, Bi,

$$Bi = \frac{\mathcal{A}i}{2\pi} \qquad (2)$$

where $i = 1, 2, ...$ and $\mathcal{A}i$ is cross-sectional area of the mini-Fermi surface of the $i-$th electronic miniband[14]; thus to each filled miniband there corresponds a period in the magnetoresistance oscillations. Parameters n_S, d and Δ of a given sample are taken to be those that give the best simultaneous agreement between all the calculated and measured SdH oscillation frequencies.

For an isolated well, Eq.(2) takes the familiar form $Bi = \pi n_S^i$, where n_S^i is the sheet carrier density in the $i-$th electronic subband. By adjusting the input parameters n_S and Δ in the theoretical model until the predicted SdH frequencies agreed with the measured ones, Koenraad determined both the sheet carrier density and the width of the donor layer in GaAs with an isolated $\delta-$well[3].

Fig. 2 shows the calculated dependence of Bi on the sheet carrier density for an isolated $\delta-$well with Δ=$0.1a_B$ ($\sim$10Å for GaAs) (solid lines) and Δ=$1.0a_B$ ($\sim$100Å for GaAs) (dashed lines). When the width of the donor layer is increased, the $\delta-$well becomes broader, consequently the energy difference between the minimum of the subbands decrease, resulting in a transfer of electrons from the subband $E1$ to $E2$ and $E3$. It is observed that the calculated SdH oscillation frequencies exhibit a substantial sensitivity to the width Δ: for a variation of Δ from $0.1a_B$ to $1.0a_B$, at $n_S = 2.0a_B$ the change in the calculated frequencies $B1$ is more than 0.7 at.unit. Considering that the Bi can be detected experimentally with an accuracy of $\pm$0.2 Teslas[3], and taking the GaAs effective mass and dielectric constant to be $m^* = 0.0665\ m_0$ and $\epsilon = 12.6$, respectively, it can be expected that the SdH analysis can produce an estimate of Δ with an uncertainty of about $\pm$5Å.

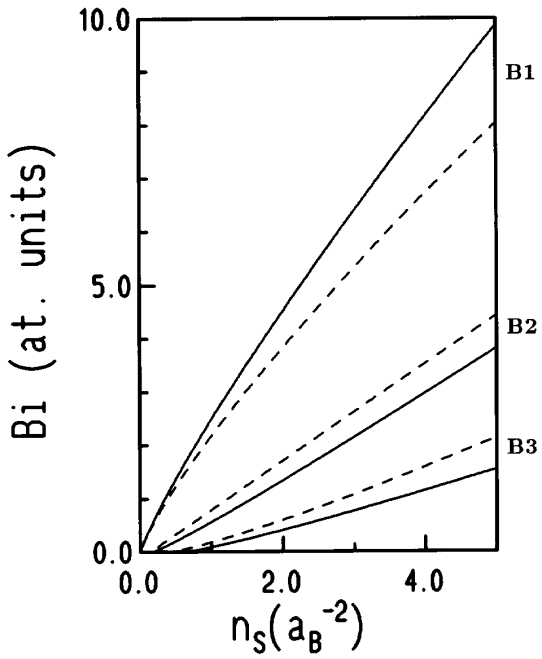

Figure 2. Calculated SdH oscillation frequencies Bi for an isolated $\delta-$well. Full lines correspond to Δ=$0.1a_B$ and dashed lines to Δ=$1.0a_B$.

Fig. 3 depicts the calculated SdH frequencies Bi as a function of n_S using a fixed value of the donor layer width, Δ=$0.2a_B$, for superlattice periods of $d = 1.5a_B$ and $d = 2.0a_B$. As the superlattice period is made shorter, it is required a higher value of doping n_S to populate the excited minibands; for this reason, as the period d is decreased, functions $Bi(n_S)$ for the excited minibands intersect the horizontal axis at higher values of n_S. Fig. 2 and Fig. 3 demonstrate that the SdH spectrum is sensitive to all the characteristic parame-

ters (n_S,d and Δ) of a $\delta-$doped superlattice, and it can in principle be used to estimate all the characteristic parameters of a given sample. In this paper, however, the period of the superlattice is obtained from CV measurements, and we limit our analysis of the SdH spectra to extract the parameters n_S and Δ only.

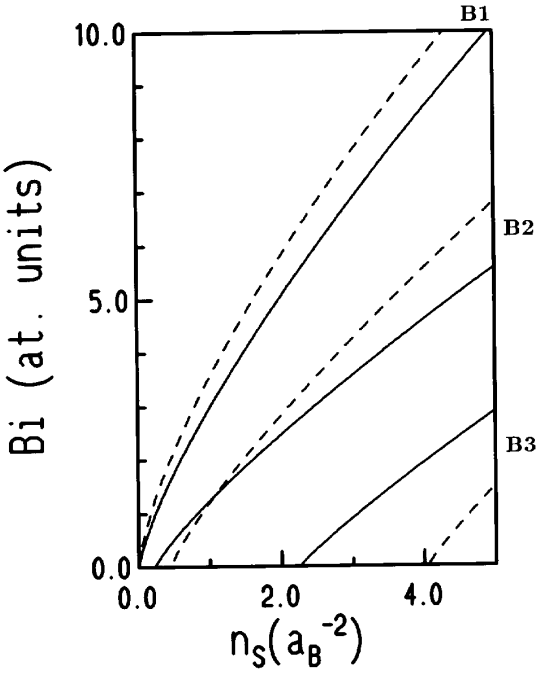

Figure 3. Calculated SdH oscillation frequencies Bi for a SL with d=2.0a_B (full curve) and d=1.5a_B (dashed curve). The calculations were done with Δ=0.2a_B.

CV profiles were calculated by resolving self–consistently the Schröedinger and Poisson equations for the superlattice under bias. The capacitance of the system at a given bias is then determined according to $C = dQ/dV$, and the CV profiles were obtained from

$$N_{CV} = 4\pi C^3 \frac{dV}{dC} \qquad (3)$$

where V is the external bias and N_{CV} is the CV concentration, which occurs at a depth $z = 1/4\pi C$ from the surface of the sample.

III. Experimental

The $\delta-$doped InP:Si structures were grown by LP–MOVPE in a AIX 200 reactor. The source materials were PH_3 (100%), trimetilindium (TMI) and silane (SiH_4) as dopant. The InP epilayers were grown on (100) Fe-doped InP substrates at 640°C and pressure 20 mbar with a growth rate of about 4Å/s. The structures consisted of a 0.4μm thick undoped InP buffer layer, the doped structure, and a cap layer of 0.06–0.07μm thickness. During the growth the $\delta-$doped plane was sinterized after the TMI flow was bypassed and the surface was PH_3 stabilized. The planar doping was accomplished by introducing SiH_4 in the gas phase.

Hall measurements at 4.2K were performed using the van der Pauw technique, and the average Hall mobility was approximately 4000 cm^2/Vs for all samples. The Shubnikov–de Haas measurements were made using a four–contact geometry; the samples were approximately square, with contacts in the corners. The magnetoresistance oscillations were studied at a fixed temperature of 4.2K in magnetic fields up to 14 Teslas. Measurements were done in the constant current mode, employing currents of 10–50 μA. Prior to the beginning of measurements the samples were irradiated with a red LED with the purpose of neutralizing the background impurities. CV measurements were performed using a PN4300 profiler. By applying a reverse bias to the Schottky contact on the surface of the sample and measuring the differential capacitance, the distribution of charge within a distance of $\sim$ 500Å from the surface can be probed[1]. To probe distances further from the surface, the sample was etched prior to the CV measurement.

IV. Results and discussion

We studied three $\delta-$doped InP samples listed in Table I. One of these samples (No.124) contained a single $\delta-$layer. The other two samples contained 20 $\delta-$layers; the sheet donor density in sample No.121 was approximately the same as in sample No.124, whereas sample No.120 had a smaller doping level. Fig 4(a) shows the Shubnikov-de Haas spectrum for sample No.124, and (b) its inverse-field Fourier transform. The peaks seen at 9.5, 22.6 and 65.6 Teslas correspond the occupation of subbands $E3$, $E2$ and $E1$, respectively. As shown by Skuras *et al*[15], the width at half maximum of a Fourier peak can be associated with the quantum mobility of the carriers in the corresponding subband; the decreasing width of the peaks as we go from $E1$ to $E2$ and $E3$ reflect an increasing mobility of the carriers, in agreement with previous observations[16,3]. This effect is responsible for a smaller uncertainty in the measured

Table I. Frequency of the oscillations in the magnetoresistance of $\delta-$doped InP:Si. The experimental values are an average of 5 measurements at 4.2K. The values of n_S and Δ and their uncertainties were estimated from the measured values of Bi.

Sample	Number of donor layers	period d (Å)	Measured $B1$	Measured $B2$ (Teslas)	Measured $B3$	Calculated $B1$	Calculated $B2$ (Teslas)	Calculated $B3$	n_S (10^{12}cm^{-2})	Δ (Å)
124	1	—	65.6 ± 1.0	22.6 ± 0.5	9.5 ± 0.1	65.2	25.4	9.3	4.94 ± 0.05	30 ± 6
120	20	270	19.6 ± 1.1	8.1 ± 0.3	—	19.6	8.1	—	1.14 ± 0.06	53 ± 15
121	20	400	64.4 ± 1.9	23.6 ± 1.2	11.3 ± 0.3	64.4	25.7	11.0	4.89 ± 0.01	39 ± 7

peak position in the Fourier transform which are associated to more excited minibands, as shown in Table I. In the SL, however, the electrons in the excited minibands are delocalized, and they interact simultaneously with several donor layers, resulting that their quantum mobilities are smaller than in the isolated $\delta-$well case[17], consequently the Fourier peaks are broader and the uncertainty in their positions is larger, as Table I shows.

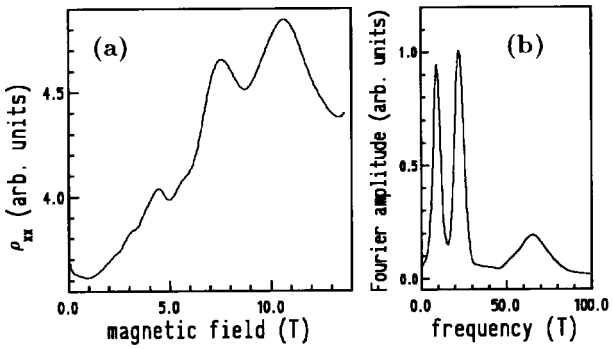

Figure 4. Shubnikov–de Haas spectrum (a) and its inverse field Fourier transform (b) for sample No.124.

In order to compare the experimental results to the theoretical calculations, the electronic effective mass and the dielectric constant for InP were taken to be equal to $m^* = 0.08m_0$ [18] and $\epsilon = 11.8$ [19] respectively. The values of n_S and Δ for each sample were taken to be equal to those that gave the least square deviation of the calculated to the experimental SdH frequencies, and the uncertainties in the values of n_S and Δ were estimated from the experimental errors in the values of Bi. The values of n_S estimated from the Shubnikov–de Haas measurements are in approximated agreement with the values of these parameters estimated from the conditions of growth. Table I summarizes the results of the experiment and calculations for all samples: a comparison of the measured SdH oscillation frequencies to the calculated ones is given, and the best-fit values of n_S and Δ are shown. The greater uncertainty in the estimated value of Δ for sample No.120 is due to the fact that this sample has a lower doping level, and for this sample only two peaks are seen in the Fourier transform of the Shubnikov–de Haas oscillations.

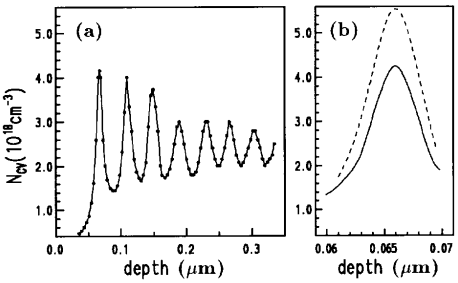

Figure 5. CV profile for sample No.121: (a) is the result obtained by alternating etching of the sample and taking a CV measurement (b) is a single CV scan which allows to probe the charge distribution around the first donor layer; the dashed line represents the theoretical CV spectrum generated by using the values of n_S and Δ obtained from the Shubnikov–de Haas spectrum.

Fig. 5(a) shows the CV profile for sample 121 obtained by alternating a CV measurement and an etching of the sample repeatedly. From the CV profile the superlattice period is determined to be 400 ± 15Å. The CV profile shown by the full curve in Fig. 5(b) was obtained by a single CV scan of the sample which was etched prior to the beginning of the measurements. The dashed curve in Fig. 5(b) is the theoretical CV spectrum for sample 121, generated with the sample parameters given in Table I and by using Eq. 3.

The width at half maximum of the CV peak of Fig. 5(b) is 70Å; the width of the theoretical spectrum, shown in Fig. 5 by the dashed line, reproduces this result, although the height of the theoretical peak is larger

than obtained experimentally. Thus, the characteristic width of the donor layer estimated from the SdH spectrum is in quantitative agreement with the value estimated from the CV spectrum.

V. Conclusions

It was demonstrated that the Shubnikov–de Haas experiment can serve the purpose of determining the characteristic parameters of a $\delta-$doped superlattice – the carrier distribution among the superlattice minibands, the width of the donor layer, and the superlattice period. In this paper we have limited the analysis of the Shubnikov–de Haas spectrum to the estimate of the sheet carrier density, n_S, and the width of the donor layer, Δ, and fixed the period of the superlattice at the value obtained from the CV measurement. The value of Δ obtained from the analysis of the SdH spectrum is in good agreement with the value predicted by the CV technique.

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