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Potential fluctuations in CdTe epitaxial layers studied by shallow donor spectroscopy in the far infrared

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Abstract
Shallow donor far infrared spectroscopy was carried out on n-type CdTe thin layers grown by molecular beam epitaxy on semi-insulating GaAs substrates. Indium doped layers of 0.5 μm thickness were deposited on a nominally undoped CdTe buffer layer with the thickness between 0.5 and 7 μm. We show that (i) the layers investigated are unintentionally doped with a native donor of an unknown origin with the chemical shift different from that of In; (ii) the shape of the spectral lines shows that the CdTe part of a structure is composed of layers characterized by either a small or a large disorder; (iii) the main sources of the disorder are structural defects originating from the CdTe/GaAs interface and propagating into CdTe layers over a distance of about 4 μm.

1. Introduction

Investigation of shallow impurities is an important part of solid state physics because it enables one to compare experimental results with a theoretical description based either on the **kp** model or on numerical studies [1]. For this reason, shallow impurity spectroscopy is a tool for testing the quality of theoretical models both for bulk semiconductors and for quantum structures. Recently, a new aspect of shallow impurity spectroscopy has emerged, stimulated by refined microscopic techniques. Nowadays application of atomic resolution microscopy enables one to investigate single impurities which opens the possibility of testing the basis of quantum mechanics by investigation of single atoms embedded in a host semiconductor [2]. For such an investigation, high quality semiconductor structures are necessary, and the present paper describes a tool for characterizing the quality of epitaxial layers with classical shallow donor far infrared magnetospectroscopy for CdTe.

Quantum structures based on CdTe are used for advanced studies in solid state physics, like investigation of the in-plane anisotropy of asymmetric quantum wells [3], properties of trions [4] and coupling of the spin of free carriers with localized magnetic moments [5]. High quality quantum structures with a minimal possible degree of disorder are necessary for such studies. In most cases, however, CdTe-based structures are grown on substrates of semi-insulating (SI) GaAs, in spite of a large lattice mismatch between the two materials, that equals 14.7%. This makes a GaAs/CdTe interface a highly disordered region with a possible destructive influence on the quality of quantum structures. Thus, it is important to avoid interface-induced disorder and to propose a method of evaluation of the disorder degree.

Typically, Hall effect measurements are used for characterization of the quality of a structure. The comparison of measured electron Hall concentration with doping level defined by the growth conditions allows us to estimate the degree of compensation. The Hall mobility gives an independent check of the level of compensation and allows for a general evaluation of the quality of the structure. A drawback of the Hall effect measurements is that the information obtained is an integral response from the part of the sample responsible for conducting the current.

In this paper we describe an alternative approach to the problem of evaluation of the quality of epitaxial layers. We describe intra-shallow donor spectroscopy measurements in

Table 1. Parameters of samples investigated. The Hall concentration n_H and mobility μ_H refer to 300 K.

Sample	Name	Dopant	d_b (μm)	d_l (μm)	n_H (10^{16} cm^{-3})	μ_H (cm^2 V^{-1} s^{-1})
06225B	A	In	0.5	0.5	—	—
06225C	B	In	3.0	0.5	1	200
03245A	C	—	5.0	—	—	—
06225A	D	In	7.0	0.5	4.8	1200

far infrared (FIR) carried out on CdTe layers. Thin layers doped with donors were grown on an undoped CdTe buffer whose thickness d_b varied from sample to sample. An SI GaAs substrate was used. We show that the shape of the spectra for the 1s–2p$^+$ intra-donor transition changes with d_b. These changes are related to the degree of structural disorder that originates from the GaAs/CdTe interface and fades out with the increased distance from the interface. The results show that investigated spectra give more detailed information about disorder than the Hall effect measurements—a spectrum clearly shows contributions from regions of a small and large electrostatic potential fluctuations which originate from this disorder.

The paper is organized in the following way. In section 2 we give some general information about fluctuations of the electrostatic potential and their role in interpretation of experimental data. The experimental details and results are described in sections 3 and 4. Section 5 is devoted to a discussion of the results obtained.

2. Fluctuations of the electrostatic potential

Fluctuations of the electrostatic potential are deviations from a perfect periodic crystallographic potential. They result from a random distribution of charged defects that break a translational invariance of the perfect crystal. Fluctuations are created, for instance, by charged impurities or dislocations. The latter are of a special interest for the present work. In the following we will consider only long range fluctuations with characteristic dimensions of several lattice constants.

Fluctuations of the electrostatic potential are of importance in interpretation of optical and conductivity properties of semiconductors and semiconductor structures. One of the first optical experiments which invoked potential fluctuations, as a necessary component of the interpretation, was carried out on CdMnSe [6]. In disordered materials, the existence of localized states at the bottom of the conduction band (CB) and appearance of the mobility edge are among the most important manifestations of fluctuations [7]. An analysis of low temperature magnetotransport experiments in SI GaAs allowed it to be proposed that the amplitude of potential fluctuations observed experimentally depends on the spatial extent of the electron wavefunction that probes the fluctuations [8]. The problem of determining the amplitude or spatial extension of fluctuations has been solved thanks to more refined experimental methods. For example, Mensz *et al* [9] determined the mean fluctuation of the average position of the electron wavefunction in a silicon inversion layer and a GaAs/GaAlAs heterostructure, by means of measurements of weak localization corrections [10] to the Drude conductivity. Mathur and Baranger [11] provided a precise relationship between that kinds of magnetoresistance measurements and the interface roughness. Bożek *et al* [12] determined amplitudes of electrostatic potential fluctuations on the surfaces of GaN epitaxial layers using a Kelvin probe scanning microscope. Potential fluctuations were also invoked to explain results of magnetospectroscopy experiments on shallow donors. Huant *et al* referred to potential fluctuations to explain the puzzling coexistence of neutral and negative donors in quantum wells [13]. Recently, it has been found in scanning tunneling microscopy studies on a set of individual donors in GaAs quantum wells that wavefunctions of a single donor are very sensitive to the local electrostatic disorder, i.e., potential fluctuations [2].

3. Samples and experiment

All samples investigated in this work were grown by a molecular beam epitaxy method. The substrate was a (001) SI GaAs wafer on which a 1 nm thick ZnTe layer and an intentionally undoped CdTe buffer layer were first deposited. A doped CdTe:In layer was subsequently grown on the buffer layer. The thickness of the buffer layer, d_b, varied from 0.5 to 7 μm in different samples. This allowed us to control the influence of the disorder that originated from the GaAs/CdTe interface on the doped layer. The doped layer thickness d_l was 0.5 μm; the indium doping levels were identical for all samples and of the order of 10^{16} cm^{-3}. More information on samples is presented in table 1.

Samples A, B and D differ in the thickness of the buffer layer only. Sample C is just a 5 μm thick not intentionally doped buffer layer. With the decrease of d_b from 7 μm (sample D) to 3 μm (sample B), both the electron concentration and mobility measured at room temperature decrease by a factor of about 5. A further decrease of d_b to 0.5 μm (sample A) makes the resistance of the sample too high for carrying out Hall effect measurements, as it is also in the case of sample C. At liquid helium temperatures, samples A, B and C were insulating. Magnetotransport studies showed that hopping is the appropriate mechanism of conductivity at low temperatures for sample D [14]. This indicates that the In concentration was smaller than the one corresponding to the Mott transition.

In magnetospectroscopy measurements, a CO_2 pumped molecular laser was a source of FIR radiation, and a superconducting coil was the source of the external magnetic field (B) up to 7 T (B was perpendicular to the sample surface). A sample was placed in a variable temperature insert and cooled down using an exchange gas. As was mentioned, at low temperatures, the resistance of samples A, B and C

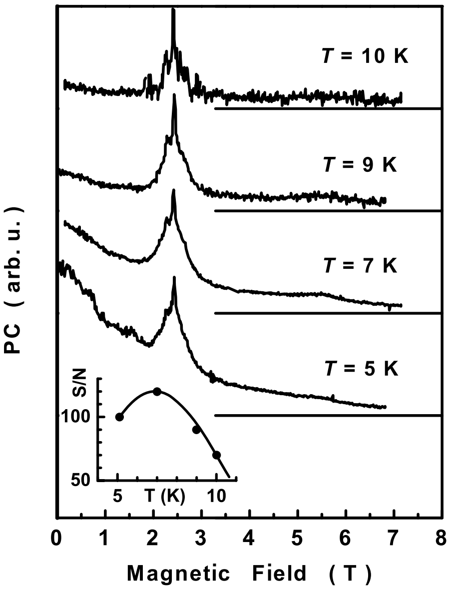

Figure 1. PC spectra for sample D at different temperatures and for $\lambda_{FIR} = 96.5\ \mu$m. No additional IR illumination was used. All spectra are normalized to the intensity of the 1s–2p$^+$ transition peak of CdTe and are shifted for clarity. Inset: estimated signal/noise ratio as a function of temperature (the solid line is a guide to the eyes).

was very high and one could not make FIR photoconductivity (PC) measurements. Therefore, the samples were additionally illuminated with an infrared (IR) light with $\lambda_{IR} = 750$ nm (the photon energy higher than the CdTe band gap). The role of the permanent IR illumination was to create mobile carriers in the conduction band and to populate shallow donors states in a stationary way. This method of carrying out FIR intra-shallow donor spectroscopy in compensated materials under permanent IR illumination was previously used in the case of shallow donors in SI GaAs [15]. Sample D exhibited a much lower resistance and therefore it was not necessary to illuminate it additionally with the IR light. In comparison, the magnetospectroscopy spectra presented for sample D were taken without (see figures 1 and 2(b)) and with (see the spectrum D in figure 3) IR illumination.

4. Results

Figure 1 shows PC spectra measured for sample D ($d_b = 7\ \mu$m) at different temperatures T. The structure positioned at about 2.5 T is due to the intra-shallow donor 1s–2p$^+$ transition in the CdTe bulk layer. The position of this peak matches the predictions from the hydrogenic model of shallow donors in CdTe [16]. The estimated signal/noise ratio (S/N) exhibits a maximum at about 7 K which is a result similar to that observed in the case of FIR measurements on shallow donors in GaAs [17]. The presence of the maximum (see the inset to figure 1) supports the interpretation underlying the role of phonons at the origin of the PC signal: the electrons excited by FIR photons from the ground to the excited state are accordingly transferred to the conduction band by a phonon cascade (the Lifshitz mechanism [18]). At low temperatures, there are not enough phonons to make the cascade efficient. On the other hand, at too high temperatures, shallow donors are thermally ionized. An interplay of these two factors leads to the maximum of the S/N dependence.

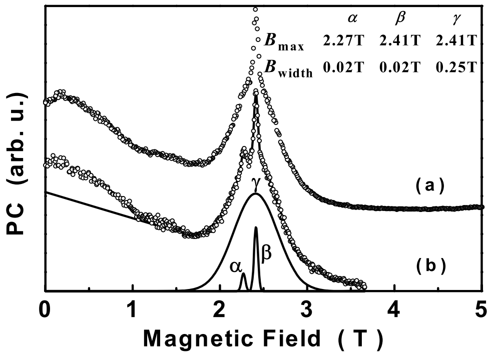

Figure 2. The 1s–2p$^+$ spectra for (a) sample C ($d_b = 5\ \mu$m) and (b) sample D ($d_b = 7\ \mu$m). $\lambda_{FIR} = 96.5\ \mu$m, $T = 7$ K. Circles: experimental data; solid line: result of deconvolution (the sum of α, β, γ peaks and a linear baseline). The position B_{max} and a halfwidth (B_{width}) of each peak are indicated. These spectra were recorded with the sweeping rate five times smaller than for spectra shown in other figures.

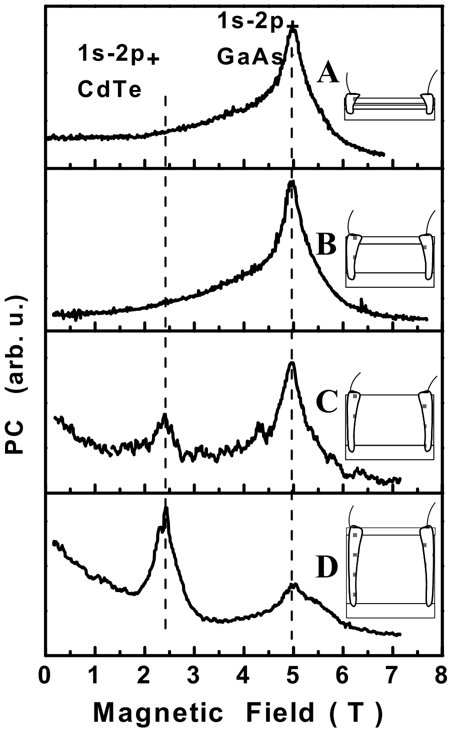

Figure 3. PC spectra for samples A, B, C, D with different CdTe buffer thicknesses for $\lambda_{FIR} = 96.5\ \mu$m, $\lambda_{IR} = 0.75\ \mu$m, $T = 7$ K. The structure of a corresponding sample is schematically presented on the right with the substrate, undoped CdTe and doped CdTe layers as well as metallic contacts.

The peak corresponding to the 1s–2p$^+$ transition can be deconvoluted into three components as shown in figure 2. In the case of the undoped buffer (sample C—see figure 2(a)), the spectrum is composed of broad and sharp peaks (marked as γ and β, respectively), centered at the same magnetic field

2.41 T; however, there is an additional peak α observed for sample D, doped with In (figure 2(b)). It is centered at $B = 2.27$ T. The difference in position is far beyond the accuracy for determining the magnetic field, which is better than 0.01 T. The aforementioned difference is due to different chemical shifts of donors [19]. We attribute the peak α to In shallow donors in a thin In doped layer, and the peaks β and γ to a native donor of an unknown origin [20]. The double structure of the native donor peak will be discussed in the next section.

It was found that the only way to deconvolute spectra was to decompose them into Gaussian peaks and a linear baseline. The solid line in figure 2(b) shows the precision of the deconvolution. The halfwidth of the narrower peaks α and β corresponds to a spectral halfwidth of about 0.2 meV. This value corresponds to the narrowest widths observed in magnetospectroscopy of shallow donors in non-compensated samples with isolated donor centers [19].

Figure 3 shows spectra measured for samples with different thicknesses of the buffer layer at the same experimental conditions with simultaneous illumination with FIR and IR light. There is only one peak in spectra (a) and (b) which corresponds to the shallow donor 1s–2p$^+$ transition in the GaAs substrate; in spectra (c) and (d) there is an additional peak corresponding to the shallow donor 1s–2p$^+$ transition in the CdTe layer. The presence of the SI GaAs-related signal indicates that both FIR and IR beams penetrate the structure down to the substrate. FIR spectroscopy of shallow donors in SI GaAs has been a subject of a number of papers [15, 21] and will not be discussed here.

All the spectra in figure 3 were registered at similar intensities of the IR illumination. The intensity of the GaAs donor peak relative to that of the CdTe donor peak decreases with increase of the CdTe buffer thickness because of (i) absorption of IR photons in the CdTe layer (fewer photons reach the GaAs substrate) and (ii) an increased volume of CdTe layers (which increases the PC due the FIR absorption in CdTe).

5. Discussion

Observation of a PC signal related to shallow donors in the SI GaAs substrate indicates that current supplying contacts pierce CdTe layers in each sample as well as reach the substrate, which is schematically shown in figure 3. Thus, the PC signal results from both the whole CdTe structure and the GaAs substrate. However, for samples A and B with the CdTe layer thicknesses of 1 μm and 3.5 μm, respectively, one observes only a GaAs-related signal under IR illumination, and no response of CdTe, despite effective absorption of the IR light in CdTe. We consider this observation as a signature of a large concentration of acceptor-like centers which effectively capture photoexcited electrons. A PC signal related to CdTe can be observed only in the case of the total CdTe thickness equal to or larger than about 5 μm (samples C and D). Let us stress that in the cases of samples C and D, the bottom part of the CdTe, of thickness of at least 3.5 μm, must be a ‘dead layer’ for the intra-donor transition, and the PC signal originates only from the upper parts of samples C and D.

These features lead us to propose the following interpretation. Due to a large mismatch between the GaAs and CdTe lattices, a GaAs/CdTe interface is crystallographically disordered. Creation of different types of defects on such interfaces was investigated using transmission electron microscopy and scanning tunneling microscopy [22, 23]. We suppose that dislocations originating from the interface and propagating into the CdTe buffer ‘transmit’ the interface disorder over a micrometer distance towards the sample top surface. The concentration of interface-related defects decreases with increase of the distance to the interface. This explains the increases of n_{H} and μ_{H} with increasing buffer thickness.

A crystallographic disorder gives rise to fluctuations of the electrostatic potential. In a simple model [24] which neglects spatial correlations of positions of charged centers, the amplitude of fluctuations increases as $N^{1/2}$, where N is the concentration of centers which create a fluctuation pattern. That is why a larger crystallographic disorder, which results in an increase of N, leads to higher potential fluctuations. On the other hand, the influence of the electric field on the width of intra-donor transitions was investigated in detail in [25], which shows that the spectral width of these transitions is enlarged by the electric field and electric field gradients (to the second order of perturbation).

In the interpretation of the present experiment we divide a sample into two parts which differ in the amplitude of the potential fluctuations. One of them is located in the proximity of the GaAs/CdTe interface, a region of a large disorder and large fluctuations. The second one is more distant from the interface and is characterized by smaller fluctuations. Disorder decrease due to the distance to the interface is caused by a decreasing concentration of mismatch dislocations penetrating the CdTe layer. That is why one can expect the crystallographic disorder within an epitaxial layer grown on a CdTe buffer to reduce with the buffer thickness. It follows that the linewidth of the transition observed for donors in CdTe will decrease if the donor distance to the interface increases.

The deconvolution of spectra shown in figure 2 is in agreement with the above reasoning. Firstly, for sample D, the line α attributed to In donors is narrow, as can be expected for donors situated far from the interface. The similar width of the native donor line β suggests that it originates from native donors which are situated at a similar distance to the interface as In donors. An equally narrow line is observed; however, also the sample C shows that the upper part of a 5 μm thick buffer is characterized by a disorder similar to that in the In doped layer in sample D.

Taking into account that no PC signal can be observed for 3.5 μm thick CdTe even with the IR illumination (sample B) we conclude that the interface-related disorder extends to a distance that is between 3.5 and 5 μm. These numbers define the maximal uncertainty limits for the distance of disorder propagation from the interface. On comparing intensities of lines of spectra (a) and (b) in figure 2, one can suggest that the upper 0.5 μm of the sample C is not disordered, which allows us to conclude that the range of propagation of the interface-related disorder is 4.0 ± 0.5 μm. Thus, the line β originates from a region of CdTe situated at a distance greater than 4 μm from the interface.

On comparing figure 2(b) and the spectrum D in figure 3 (obtained without and with the IR illumination, respectively), we notice that the IR light does not change the halfwidth of the peak γ. We conclude that the intensity of the IR illumination is too weak to generate a concentration of free carriers high enough to influence the screening of fluctuations. We note, however, weak changes of the low B part of the spectra related to the IR illumination—the broad structure existing between 0 and 1 T seen in figure 2(b) and absent in spectrum D in figure 3. This effect, however, was not investigated in detail.

Far infrared Fourier spectroscopy experiments on sample D (and other CdTe layers deposited on a GaAs substrate, not investigated in this paper) were described in [26]. It was found that changes of the conductivity of the CdTe layer were related to heating of the CdTe and GaAs layers by means of FIR photon absorption. This bolometric effect showed a spectral dependence related to the phonon density of states in CdTe and GaAs. The influence of the bolometric effect on photoconductivity spectra was also discussed in [27]. The possibility of observing the bolometric effect in [26] was connected with a small activation energy ΔE of the conductivity in the samples investigated. The magnetoresistance measurements [14] showed that the hopping conductivity at liquid helium temperatures is characterized by $\Delta E \approx 1$ meV, which means that even a very small increase of the lattice temperature can lead to observable conductivity changes.

In our experiments, one can expect two kinds of contributions due to the bolometric effect. The first one is caused by the absorption of IR radiation in CdTe and GaAs layers. The heating caused by this absorption, however, is not relevant because: (i) owing to a lock-in technique used in measurements, the signal analyzed is related solely to the chopped FIR radiation superimposed on a constant IR background; (ii) IR photon energy is far beyond lattice-related resonances of CdTe and GaAs and therefore IR-related heating is not expected to generate resonant features at the magnetic field applied. The second contribution can be related to a resonant (in magnetic field) heating caused by 1s–2p$^+$ absorption. The photoconductivity signal observed is proportional to changes of the conductivity $\Delta\sigma \sim \Delta n\mu + n\Delta\mu$, where n and μ are the concentration and mobility of the current-carrying electrons, respectively. The resonant heating influences both terms and can be considered as one of the mechanisms increasing the photocurrent without changing its spectral dependence.

The above analysis shows that shallow donor magnetospectroscopy allows us to trace a decrease of disorder degree with increase of the distance from the substrate/layer interface. A conclusion resulting from this investigation shows that the necessary thickness of the CdTe buffer layer on which quantum structures should be grown in the case of SI GaAs substrates is at least 5 μm. Similar measurements can be carried out in the case of other II–VI or III–V systems as a useful investigation to be done in order to optimize the quality of quantum structures.

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