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Anomalous behavior of the Fermi energy in heavily tin-doped InGaAs

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Abstract. We have measured the dependence of the Fermi energy on carrier concentration in Sn doped InGaAs at 4.2 K and 300 K. At 4.2 K the Fermi energy was measured by photoluminescence spectroscopy, and at 300 K it was deduced from transport measurements of thermionic emission. In both cases the dependence of the Fermi energy on the mobile electron concentration, measured by Hall effect, strongly deviates from standard theoretical predictions, and the deviation increases with concentration. The most striking observed anomaly is the near saturation of the Fermi level when the Hall concentration exceeds 10^{19} cm^{-3}.

PACS. 79.40.+z Thermionic emission – 73.40.-c Electronic transport in interface structures – 73.40.Kp III-V semiconductor-to-semiconductor contacts, p-n junctions, and heterojunctions

1 Introduction

The study of electronic interactions and their effect on the ground state of the electronic system are fundamental issues in condensed matter physics. These interactions are crucial to the understanding of a wide range of phenomena. A prime example is the electron-electron exchange interaction in the interacting electron gas [1,2] which accounts for metallic binding.

Although the importance of interactions is widely recognized, electronic systems can often be treated in the framework of non-interacting quasi-particles. Such is the case of the low-density electron gas that is formed in doped semiconductors. For this system, relatively minor corrections are believed to be necessary to account for the effects of interactions. Thus, inclusion of the exchange interaction [3] results only in a slight alteration of the Fermi energy. For the most studied situation with relatively low doping levels ($n < 1 \times 10^{18}$ cm^{-3}), there is no experimental evidence for any deviation from this assumption. This may not hold indefinitely, however, as the doping level and carrier density are increased.

Heavy doping of a semiconductor with a single type of carrier (electrons or holes) is a technologically challenging task. Studies of such samples have so far been rather limited and mostly device-oriented. Nevertheless, certain puzzling anomalies have been seen. Thus, charge injection transistors employing InGaAs/InAlAs heterojunctions with carrier densities up to $n = 6 \times 10^{19}$ cm^{-3} functioned normally at both room and cryogenic temperatures [4]. Despite the fact that the estimated Fermi energy in these samples exceeded the value of the conduction band discontinuity (0.5 eV), there was no evidence of excessive thermionic emission across the junction due to a vanishing barrier. This suggests a substantial lowering of the Fermi level owing to effects that have not been taken into account.

An alternative way to achieve high carrier densities in semiconductors is to use optical excitation, which has been used extensively to create and study dense electron-hole populations in intrinsic semiconductors [5]. While the attractive Coulomb interaction between electrons and holes manifests itself already at vanishing e-h pair densities, in the form of excitons [6] and the density-dependent band gap renormalization [7], strong modifications of the e-h system occur under conditions of high excitation densities [5]. Such observations provide further motivation for the study of heavily-doped semiconductors, where only one type of mobile carrier exists while the neutralizing positive charge resides in fixed dopant ions.

In this paper we use two complementary experimental techniques to follow the change of the Fermi level with carrier density in heavily tin-doped InGaAs/InAlAs heterojunctions. For our room temperature experiments we employ a novel transport technique, while measurements at 4.2 K are performed by standard photoluminescence spectroscopy, which is established and ideal for low-temperature measurements. In both cases we find a striking anomaly, in the form of near saturation of the

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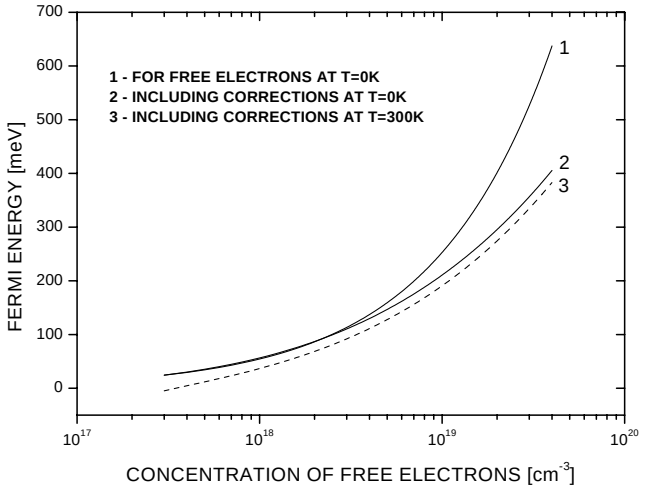

Fig. 1. Theoretical dependence of Fermi energy on carrier concentration in heavily doped InGaAs.

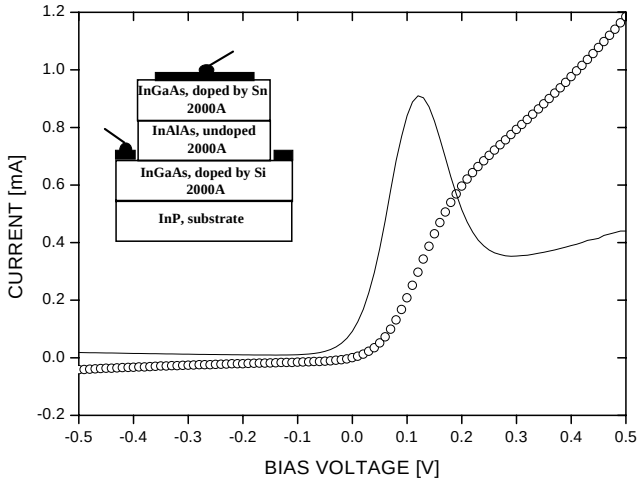

Fig. 2. Typical experimental I–V curve and its derivative for heterojunctions with Sn-doped semiconductors. The inset shows the sample cross-section and contacts used for I–V measurements.

Fermi level, when the concentration of electrons (deduced from the Hall conductivity) exceeds $n = 1 \times 10^{19}$ cm^{-3}.

Figure 1 shows the theoretical dependence of the Fermi energy on carrier concentration for the range covered by our experiments. The figure shows data for free electrons at $T = 0$, as well as data for $T = 0$ and $T = 300$ K that takes into account the electron-impurity interaction, the electron-electron exchange interaction [3] and the band nonparabolicity [8].

2 Experiment

Our samples, grown by molecular-beam epitaxy (MBE), are shown schematically in the inset of Figure 2. They have a fixed low $n_1 \approx 5 \times 10^{17}$ cm^{-3} carrier concentration in the bottom Si-doped InGaAs layer, a fixed chemical composition of the barrier and a variable carrier concentration n_2 in the top InGaAs layer, doped by Sn in the range n_2: $10^{18} \div 4 \times 10^{19}$ cm^{-3}. Standard photolithographic techniques were used to fabricate samples with Hall bar geometry (not shown) and two-terminal small area vertical junctions (see inset of Fig. 2). Separate shallow ohmic contacts were made to both the top and the bottom InGaAs layers in both Hall bar and junction geometries. The Hall bar geometry samples were employed for carrier density measurements in both layers while the junction geometry was used for I–V characteristics measurements.

Hall effect measurements were performed by the standard 4-terminal lock-in amplifier method at room temperature and low magnetic field (in the linear regime). The results confirmed that the electron density in the top InGaAs layer accurately followed the MBE calibrated Sn-donor concentration for all samples. It was also verified that the carrier concentration in the bottom InGaAs for all samples remained fixed at about 5×10^{17} cm^{-3}.

The novel transport technique [9] that we use for room-temperature measurements is based on studying thermionic transport between two semiconductor layers, one of which has a known Fermi energy. Traditional transport techniques for E_f determination rely on measurements of the activation energy of thermionic current from its temperature dependence. Such techniques are not very accurate, being limited by an uncertainty in the height of the potential barrier under particular experimental conditions. In contrast, the new technique [9] is insensitive to the height of the potential barrier and is based on the fact that under certain well-defined experimental conditions the I–V characteristic has an inflection point at the voltage V such that $eV = \Delta E_\mathrm{f}$, where ΔE_f is the difference in Fermi energies of the semiconductors on both sides of the barrier. This result is always true for "ballistic" barriers (*i.e.*, those narrower that the electron mean free path), and has been shown [9] to remain valid for wider ("diffusive") barriers, provided that the barrier contains a certain (small) amount of uncompensated positive fixed charge. In the latter case, the $\mathrm{d}I/\mathrm{d}V$ exhibits a sharp maximum at $V = \Delta E_\mathrm{f}/e$ enabling one to quantify the unknown E_f in terms of that on the reference side.

Inasmuch as the carrier concentration in the reference layer is low, we can rely on theoretical calculations of its Fermi energy [3]. Measuring the position of the maximum of $\mathrm{d}I/\mathrm{d}V$ we can hence determine the Fermi energy of the heavily doped semiconductor layer. It should be emphasized that although the I–V curve depends strongly on such factors as the barrier width and height, the electron mean free path, and the precise charge distribution inside the barrier, position of the peak in $\mathrm{d}I/\mathrm{d}V$ remains fixed by the Fermi level difference.

I–V characteristics of the junctions were measured in a 2-terminal configuration using HP 4145B Semiconductor Parameter Analyzer. A typical I–V curve of the junction is shown in Figure 2 for the sample with $n_2 = 3.6 \times 10^{19}$ cm^{-3}. The derivative of the curve $\mathrm{d}I/\mathrm{d}V$ exhibits a sharp maximum at $V = 120$ meV. Since ballistic transport is not expected through a 2000 Å barrier at room temperature, the appearance of the sharp peak must

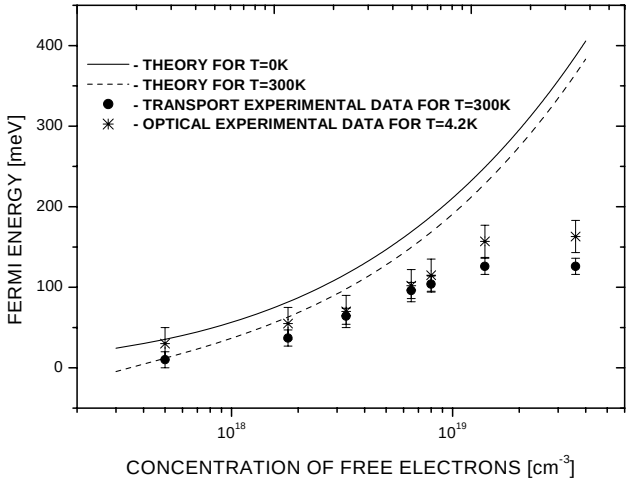

Fig. 3. Experimental dependence of Fermi energy on carrier concentration in heavily doped InGaAs.

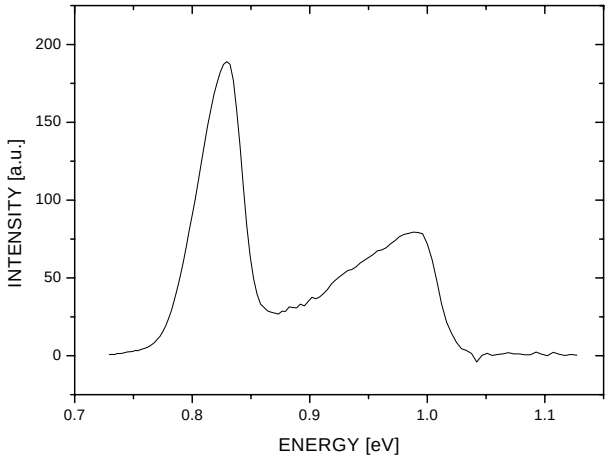

Fig. 4. Typical photoluminescence spectrum.

be due to the presence of positive charge in the barrier. While no charge was deliberately introduced into the barrier, a small amount of Sn may diffuse into it. Indeed, Sn is known to be a highly mobile dopant [10]. The actual amount of positive charge in the barrier is unimportant, as long as it exceeds 5×10^{15} cm^{-3} on average, which corresponds to a sheet concentration of 1×10^{11} cm^{-2}. Such a concentration is quite plausible [10], although we could not verify it by Secondary Ion Mass Spectroscopy (SIMS), which has a detection limit of about 1×10^{17} cm^{-3}. Thus, while in earlier studies on Si-doped samples the required positive charge was introduced intentionally in the barrier [9], for structures doped with Sn the charged barrier is obtained "for free" due to diffusion of Sn from the adjacent doped layer.

Taking the Fermi energy of the bottom layer at room temperature to be $E_{f_1} = 10$ meV, we obtain $E_{f_2} = 130$ meV for the top layer of the sample whose I–V is shown in Figure 2. Similar analysis for all measured samples results in a plot $E_f = E_f(n)$ which is shown in Figure 3. Deviation of the experimental data points from the theoretical line is quite evident. Although at low concentrations (less than 1×10^{19} cm^{-3}) the experimental data are already below the predicted theoretical curve, the general trend is that E_f increases with concentration as expected. However, at concentrations above 1×10^{19} cm^{-3} one clearly observes saturation. This result is surprising, since it contradicts the standard theory. On the other hand, it explains the non-leaky behavior of similarly doped charge injection transistors [4]. Such discrepancies have not been reported for Si doping of InGaAs, due to the inability to introduce high levels of doping in MBE growth of the material. For moderate levels of doping, up to 3×10^{18} cm^{-3}, the measured E_f is in agreement with theoretical predictions [9].

One possible origin of the observed anomaly could be associated with the diffusion of Sn and its segregation towards the surface. This could certainly cause some depletion of dopants at the InGaAs/InAlAs upper interface resulting in a band bending near the barrier interface and a reduced separation E_f from the Fermi level to the bottom of the conduction band. Since the Hall effect would not be affected by dopant redistribution within the layer, such a depletion could in principle account for the anomaly shown in Figure 3, provided that the concentration at the InGaAs/InAlAs interface is saturated at about 1×10^{19} cm^{-3}. In order to confirm or eliminate this hypothesis, we studied the distribution of Sn by SIMS analysis on the sample with Sn concentration of 4×10^{19} cm^{-3} (according to MBE calibration), which shows a mobile electron concentration of $n = 3.6 \times 10^{19}$ cm^{-3} (according to Hall measurements). We found that while the average concentration of Sn is consistent with the MBE calibration and Hall measurements, there is only a small linear variation of the Sn concentration in InGaAs from 3×10^{19} cm^{-3} at the barrier interface to 5×10^{19} cm^{-3} at the top of the layer, over the total distance of 2000 Å. The observed variation of Sn concentration and its depletion at the barrier interface by about 25% of the average are far too small to account for the saturated low value of measured E_f. As mentioned before, no Sn was detected inside the barrier, which implies a concentration of less than $n = 1 \times 10^{17}$ cm^{-3}. We therefore conclude that the main reason for the linear variation in Sn concentration is segregation towards the surface, and that this variation cannot account for the observed saturation of E_f and its strong deviation from the theoretical curve.

In order to determine the E_f at 4.2 K we measured the photoluminescence spectrum of samples taken from the same wafers. Each sample was mounted in vacuum on the cold finger of a continuous flow cryostat, and illuminated by the focused beam of a laser. We used both pulsed radiation from a Ti:Sapphire laser at 800 nm, and monochromatic doubled-YAG at 532 nm. In both cases we estimate the optically excited electron-hole density to be below $n = 5 \times 10^{17}$ cm^{-3}. The photoluminescence signal was collected at 90 degrees to the incoming beam, and measured with a 50 cm monochromator and an IR detector. A typical spectrum of the observed luminescence is shown in Figure 4. The low-energy peak corresponds to recombination of carriers in the vicinity of $k = 0$. This

is in agreement with the fact that, on the time scale of the measurements, all photoexcited holes relax to $k = 0$ and most of the recombination occurs at the band edge. The position of the peak closely agrees with the known bandgap of InGaAs at 4.2 K, $E_G = 0.82$ eV. The broad high-energy shoulder of the spectrum corresponds to recombination of higher-energy electrons in the Fermi sea with the holes at $k = 0$. Because of the increasing density of states occupied by electrons with higher wavenumber, the intensity of luminescence in the shoulder is slowly increasing towards a maximum at the energy corresponding to electronic transitions from the Fermi level, where a sharp cutoff is observed. Further enhancement close to the Fermi level may result from the Fermi edge singularity effect (Mahan exciton) [11]. Although recombination with holes at $k = 0$ is not allowed for electrons at $k > 0$ in a perfect crystal, due to the dipole selection rules, it may occur in a real sample due to the quantum uncertainty of the hole wavenumber, induced by localization. This may partly explain why the low energy peak in the photoluminescence spectrum is strong: although the density of states near $k = 0$ is small, the dipole matrix element for recombination with the holes at the zone center is large. Another contribution to the low energy peak in the photoluminescence data may come from the emission of the lower, Si-doped layer. The fact that the Fermi level in the latter is small compared to the photoluminescence linewidth makes the two contributions indistinguishable. Hence the difference between the two peaks in the spectrum measures E_f in the top layer, up to an error on the order of E_f in the bottom layer. For the example shown in Figure 4 we find $E_f = 163$ meV. Similar results for all measured samples yield a plot $E_f(n)$ shown in Figure 3 together with the room-temperature results.

We see that the cryogenic E_f is higher than that at 300 K, as should be expected. However, the discrepancy with the theoretical predictions for 4.2 K remains strong. In particular, the salient feature of Fermi level saturation above 1×10^{19} cm^{-3} persists to cryogenic temperatures.

3 Conclusion

In conclusion, we have investigated the dependence of E_f on the mobile carrier concentration in heavily Sn doped InGaAs layers by two independent techniques at room and helium temperatures. We found the Fermi level to be generally below the curve predicted by current theory, even when the latter includes the effects of electron-impurity interaction, the electron-electron exchange interaction and the band nonparabolicity. Furthermore, at concentrations exceeding 1×10^{19} cm^{-3} the dependence of E_f on the mobile carrier concentration saturates altogether at a value of about 130 meV.

The discrepancy between our measurements and the best available current theory is as high as 0.25 eV at highest levels of doping. Compared to free-electron estimates of the Fermi level, the discrepancy is still higher, exceeding 0.5 eV. All known corrections due to the nonparabolicity and Coulombic interactions and correlations bring the theory only half way toward the experimental values measured in this work. Although some redistribution of Sn in the doped InGaAs layer was observed, it cannot account for the observed saturation of E_f and its strong deviation from the theoretical curve.

We believe our results are convincing enough to encourage the development a new theoretical model appropriate to heavily doped semiconductors. At the same time there is an experimental challenge to find out whether the observed anomaly is exhibited by a large class of semiconductors and dopants or is peculiar to tin-doped InGaAs.

It should be noted, moreover, that the observed saturation of the Fermi level at high carrier concentrations calls for a thorough revision of our picture of screening in heavily doped semiconductors. Indeed, our results imply that local fluctuations of the impurity concentration produce no accompanying potential fluctuations in heavily doped semiconductors, an effect which should have pronounced manifestations, *e.g.*, in the deep tails of the interband optical spectra of heavily doped semiconductors [3].

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