SATURATION OF FERMI ENERGY IN HIGHLY Sn DOPED InGaAs

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We describe a method of Fermi energy measurement based on the analysis of thermionic emission and diffusion over a barrier with a build-in charge. The method was successfully tested by measuring the Fermi energy in GaAs. In addition, this method was applied to measure the Fermi energy in heavily Sn doped InGaAs. The dependence of the Fermi energy determined by thermionic emission on carrier concentration measured by Hall effect strongly deviates from standard theoretical predictions. The most striking observed anomaly is the near saturation of the Fermi level at a value $E_f \simeq 130$ meV when the mobile carrier concentration exceeds 10^{19} cm⁻³. Our results call for a thorough re-examination of the existing theory.

1 Description of the Method

In general, electronic current over a barrier depends on its height E_b , width w, the electronic mean free path l, the temperature T, and the Fermi energies E_{f_1} , E_{f_2} in semiconductor layers on both sides of the barrier (where $E_f \equiv E_F - E_C$ is defined relative to the conduction band edge in each semiconductor, see Fig. 1(a)).

As will be shown below (eq. (1) for $w \to 0$) the I-V characteristic for a ballistic barrier, i.e. for a barrier with w < l, has a remarkable feature that the derivative dI/dV exhibits a pronounced maximum when the bias voltage $eV \equiv E_{F_2} - E_{F_1}$ equals the Fermi level difference, $eV = E_{f_2} - E_{f_1}$. The latter condition is equivalent to $E_{C_1} = E_{C_2}$ ("flat bands"). Thus, for a ballistic barrier, one can easily extract from the I-V characteristic the Fermi energy for one of the semiconductors, provided that the Fermi energy of the other semiconductor is known.

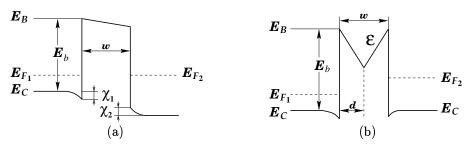


Figure 1: (a) Potential offsets near the barrier. (b) V-shaped potential barrier with electric field \mathcal{E} .

Unfortunately, in order that transport over the barrier was ballistic at room temperature, the barrier must be so narrow that tunneling and field emission components of the total current cannot be ignored. Because of this complication, it is impossible to determine E_f from the dI/dV curves in narrow barriers. On another hand, for wide barriers (l < w), where the tunneling and field emission contributions can be ignored, the I-V curves do not exhibit a sharp maximum in dI/dV at $eV = E_{f_2} - E_{f_1}$ and therefore these curves can neither be employed for Fermi energy measurements. As a result, the temperature dependence of thermionic current, which is perhaps the simplest to measure transport characteristic, has only been used for measurements of the barrier height (if the Fermi energy is known) or for measurements of the Fermi energy (if the barrier height is known).

In the following we describe a new method for the Fermi energy determination. It is based on thermionic emission and diffusion through a wide (w>l) but charged barrier. We shall demonstrate that the I-V characteristics for such a barrier are similar to those for a ballistic barrier in that the derivative dI/dV has a pronounced maximum at $eV=E_{f_2}-E_{f_1}$.

It was shown by the authors ¹ that the solution of the drift-diffusion equation with the boundary conditions on the concentration at both interfaces between the barrier and the semiconductors gives the following expression for the current in the heterojunction as a function of the bias voltage:

$$J = \frac{N_c e^{-\frac{E_b - \chi_2(V) - E_{f_2}}{kT}} (1 - e^{-\frac{eV}{kT}})}{\frac{1}{ev_R} (1 + e^{-\frac{eV^*}{kT}}) + \frac{\alpha w}{e\mu V^*} (1 - e^{-\frac{eV^*}{kT}})}$$
(1)

where V^* is the potential drop, $eV^* \equiv E_B(w) - E_B(0) = eV - (E_{f_2} - E_{f_1}) - \chi_1(V) - \chi_2(V)$, $\chi_1(V)$ and $\chi_2(V)$ are the band bendings near the barrier, μ is the mobility of electrons in the barrier and N_C is the densities of states of

electrons in the semiconductor layer.

The derivative dJ/dV of the eq.(1) has a pronounced maximum at $eV = E_{f_2} - E_{f_1}$ only for ballistic barriers $(w \to 0)$.

In full analogy with the previous case, for the barrier of width w=2d with a positively charged plane in the middle of it which results in a V-shaped potential of the barrier with electrical field \mathcal{E} (see Fig. 1(b)) the solution of thermionic diffusion equations gives the following expression for the current density as a function of applied voltage V:

$$J = \frac{\frac{e\mu\mathcal{E}_1\mathcal{E}_2}{\mathcal{E}_2 - \mathcal{E}_1} \left(B_2 e^{-\frac{e\mathcal{E}_2 d}{kT}} - B_1 e^{-\frac{e\mathcal{E}_1 d}{kT}} \right)}{1 - \frac{e\mu\mathcal{E}_1\mathcal{E}_2}{\mathcal{E}_2 - \mathcal{E}_1} \left(A_2 e^{-\frac{e\mathcal{E}_2 d}{kT}} - A_1 e^{-\frac{e\mathcal{E}_1 d}{kT}} \right)} , \tag{2}$$

where $\mathcal{E}_1 = -\mathcal{E} + rac{V^*}{w}; \mathcal{E}_2 = \mathcal{E} + rac{V^*}{w};$

$$A_1 = \frac{1}{\alpha e v_R} (1 - \frac{v_R \alpha}{\mu \mathcal{E}_1}); A_2 = -\frac{1}{\alpha e v_R} (1 + \frac{v_R \alpha}{\mu \mathcal{E}_2}) e^{\frac{e \mathcal{E}_2 w}{kT}}$$
(3)

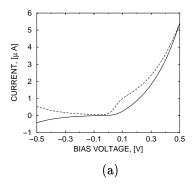
$$B_{1} = \frac{N_{c}}{\alpha} e^{-\frac{E_{b} - E_{f_{1}} + \chi_{1}}{kT}}; B_{2} = \frac{N_{c}}{\alpha} e^{-\frac{E_{b} - E_{f_{2}} - \chi_{2}}{kT}} e^{\frac{e\varepsilon_{2}w}{kT}}$$
(4)

Here $\alpha \equiv N_C^{(b)}/N_C = (m_b^*/m^*)^{3/2}$, $v_R = \sqrt{kT/2\pi m_b^*}$ is the Richardson velocity, corresponding to the effective mass of electrons in the barrier 2 (N_C and $N_C^{(b)}$ are the densities of states and m^* and m_b^* the effective masses of electrons in the semiconductor layers and in the barrier respectively). \mathcal{E} is positive for positively charged barrier.

For a neutral barrier $(\mathcal{E}=0)$ expression (2) reduces to (1). Thus, when $\mathcal{E}=0$ and $\mu \ll \frac{ev_R\alpha w}{kT}$ (the mean free path is shorter than the width of the barrier) the current is significantly suppressed relatively to its ballistic value, and dI/dV is not peaked at $eV=E_{f_2}-E_{f_1}$, as shown in Fig. 2(a).

and dI/dV is not peaked at $eV=E_{f_2}-E_{f_1}$, as shown in Fig. 2(a). For a diffusive and charged $(\mathcal{E}\neq 0)$ barrier the thermionic current behaves similar to the ballistic case when $|\mathcal{E}|\geq \frac{\alpha v_R}{\mu}$ and the dI/dV has a pronounced maximum at $eV=E_{f_2}-E_{f_1}$. Fig. 2(b) shows that the peak at the dI/dV is still well resolved even when $|\mathcal{E}|=\frac{\alpha v_R}{\mu}$. The condition $|\mathcal{E}|>\frac{\alpha v_R}{\mu}$ is equivalent to $l\mathcal{E}>kT/e$, as discussed in detail by Grinberg and Luryi 3 .

In order to check these equations and their utility for Fermi energy measurement, we have grown by molecular-beam epitaxy (MBE) two samples containing GaAs/Al_{0.3}Ga_{0.7}As heterojunction as shown in the insets of Fig. 3(a),(b). As seen from the figures, the samples are almost identical ($N_D = 3 \times 10^{18} \text{ cm}^{-3}$ in the top GaAs layer and $N_D = 1 \times 10^{18} \text{ cm}^{-3}$ in the bottom one) with the only difference being in the barriers. In sample b) δ -doping of Si with sheet carrier concentration $\sigma = 1 \times 10^{12} \text{ cm}^{-2}$ was introduced in the middle of the



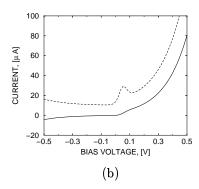


Figure 2: (a) Theoretical I-V curve (solid line) and its $\mu=500~\mathrm{cm^2/Vsec},~E_b=300~\mathrm{meV},~E_{f_1}=40~\mathrm{meV}, E_{f_2}=90~\mathrm{meV}$ at $T=153~\mathrm{K}.$ (b) Theoretical I-V curve (solid line) and its derivative (dashed line) for charged barrier with $\mu=500~\mathrm{cm^2/Vsec},~E_b=300~\mathrm{meV},~\mathcal{E}=2\times10^4~\mathrm{V/cm},~E_{f_1}=40~\mathrm{meV},~E_{f_2}=90~\mathrm{meV}$ at $T=167~\mathrm{K}.$

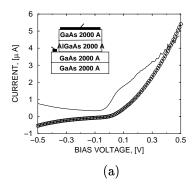
barrier. The highest possible field in the barrier that can be produced by Si donors is given by $\mathcal{E}=(E_B-E_D)/d$, where E_D is the donor energy level. For Si in Al_{0.3}Ga_{0.7}As we obtain $\mathcal{E}\approx 2\times 10^4$ V/cm, which corresponds according to Gauss' law $\mathcal{E}=\frac{e\sigma}{2\epsilon}$ to $\sigma\approx 2.7\times 10^{11}$ cm⁻². It means that roughly 1/4 of Si donors are ionized.

Standard photolithographic technique was used to fabricate two-terminal small area vertical junctions (see the insets of Fig. 3(a),(b)). Separate shallow Ohmic contacts were provided to top and bottom GaAs layers. The junctions were utilized for I-V characteristics measurements.

I-V characteristics of the junctions were measured at $T\approx 160~\mathrm{K}$ in a 2-terminal configuration, using HP 4145B Semiconductor Parameter Analyzer. This temperature was chosen in order to diminish the contribution of the ohmic contacts resistance to the junction resistance, which were comparable at room temperature.

The I-V curve of the junction with uncharged barrier is shown in Fig. 3(a). The shape of the curve is similar to the shape of the theoretical curve (Fig. 2(a)), which is plotted for the parameters of our structure. The derivative dI/dV does not exhibit any local maximum.

At the same time, as expected, dI/dV curve for the case of charged barrier shows a well pronounced peak at $V\approx 50$ meV (see Fig. 3(b)). Moreover, the shape of the I-V curve is similar to the one depicted in Fig.2(b). Although the variation in all structure parameters used in the theoretical curve would drastically change the shape of the I-V characteristic the peak in dI/dV and



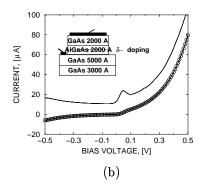


Figure 3: (a) Experimental curve (circles) and its derivative for uncharged barrier. The inset - vertical junction for *I-V* measurements and sample structure with undoped barrier. (b) Experimental curve (circles) and its derivative for charged barrier. The inset - vertical junction for *I-V* measurements and sample structure with doped barrier.

its position will stay in place as long as $|\mathcal{E}| \geq \frac{\alpha v_R}{\mu}$ and $E_{f_2} - E_{f_1}$ is fixed. In our structures with charged barriers the condition $|\mathcal{E}| \geq \frac{\alpha v_R}{\mu}$ is satisfied for $\mu \geq 500 \text{ cm}^2/\text{V}$ sec. Note, that in order to observe "real" ballistic transport in our structures the requirement for the mobility in the barrier would be $\mu \gg 3500 \text{ cm}^2/\text{V}$ sec, which is hard to meet. We do not know the exact value of the mobility in our AlGaAs barriers. However, $\mu \geq 500 \text{ cm}^2/\text{V}$ sec is reasonable value at $T \approx 155 \text{ K}$ for the AlGaAs grown by MBE. We would like to emphasize again that the exact value of μ is of no importance as long as it exceeds $500 \text{ cm}^2/\text{V}$ sec.

The position of the peak in dI/dV in Fig.3(b), namely $eV \approx 50$ meV is consistent with the value $E_{f_2}-E_{f_1}=54$ meV where $E_{f_1}=38$ meV for $n_1=1\times 10^{18}$ cm⁻³ and $E_{f_2}=92$ meV for $n_2=3\times 10^{18}$ cm⁻³ (these values of carrier concentrations were confirmed by standard Hall measurements). It proves that the thermionic emission through a charged wide barrier can be utilized as a new simple experimental tool for measurements of the Fermi energy in a variety of semiconductors.

2 Measurements of the Fermi Energy in heavily Sn doped InGaAs

We have applied the above described method to measure the Fermi energy in heavily Sn doped InGaAs.

The nearly-free electron model predicts a rather low density of states and hence a high Fermi energy for heavily doped InGaAs due to its low effective

electron mass. For example, an electronic density of $n=3\times 10^{19}~{\rm cm^{-3}}$ results in the Fermi energy, $E_f\approx 0.5~{\rm eV}$. Taking into account the electron-impurity interaction, the electron-electron exchange interaction ⁴ and nonparabolicity of the band ⁵ one obtains a lower value for the Fermi energy. Although these corrections are larger for higher electron concentrations, see Fig. 4(b), still the Fermi energy will exceed 0.5 eV for $n>6\times 10^{19}~{\rm cm^{-3}}$. This value of 0.5 eV is very significant because it equals the conduction band discontinuity at InGaAS/AlInAs heterojunction. Therefore, all types of electronic devices employing this heterojunction at $n>6\times 10^{19}~{\rm cm^{-3}}$ and which require the existence of the barrier in the junction should be expected to fail. However, such devices grown at Bell Laboratories ⁶ exhibit normal performance for even higher values of n without any indication of barrier disappearance. Our investigation is aimed at quantification of the dependence of the Fermi energy on carrier concentration in heavily doped InGaAs.

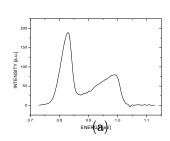
We grew by molecular-beam epitaxy (MBE) a set of heterojunctions schematically shown in the inset of Fig. 4 with fixed low $n_1\approx 5\times 10^{17}~{\rm cm}^{-3}$ carrier concentration in the first (bottom) InGaAs, fixed chemical composition of the barrier and a variable doping concentration n_2 in the second (top) InGaAs layer in the range $n_2:10^{18} \div 4\times 10^{19}~{\rm cm}^{-3}$. Each of the layers had the width of 2000Å. The barrier layer was not doped artificially because in heavily Sn doped sandwiches there is no need to do that since Sn is well known to be a highly mobile dopant ⁷ and the diffusion of a small amount of Sn into the barrier during a growth provides charge sufficient to observe the above described feature of charged barrier. It can be estimated that as little as $1\times 10^{11}~{\rm cm}^{-2}$ of ionized Sn donors introduced into the barrier would yield the condition $|\mathcal{E}|\gg \frac{\alpha v_R}{\mu}$ in our structure. It is quite plausible that the barrier is doped on average at $5\times 10^{15}~{\rm cm}^{-3}$ which for a 2000Å wide barrier is equivalent to a sheet concentration of $1\times 10^{11}~{\rm cm}^{-2}$.

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, charge distribution inside the barrier, etc., the peak in dI/dV and its position will stay in place as long as $|\mathcal{E}| > \frac{\alpha v_R}{\mu}$.

I-V characteristics of the junctions (see inset of Fig. 4(a)) and carrier concentration in both top and bottom layers were measured using the same technique as described in Sec. 1. It was particularly verified that the carrier concentration in the bottom InGaAs for all samples remained fixed at about $5\times 10^{17}~{\rm cm}^{-3}$. Typical I-V curve of the junction is shown in Fig. 4(a) for the sample with $n_2=3.6\times 10^{19}~{\rm cm}^{-3}$. The derivative of the curve dI/dV exhibits a sharp maximum at $V=120~{\rm meV}$. This "ballistic" like feature of the I-V indicates on the presence of a positive charge in the barrier, as expected for

Sn doped structures.

Taking the Fermi energy of the bottom layer at room temperature to be $E_{f_1}=10~{\rm meV}$ (for low concentrations one can rely on theoretical calculations of the Fermi energy, see Fig. 4(b)) we obtain $E_{f_2}=130~{\rm meV}$ for the top layer of sample, whose I-V is shown in Fig. 4(a). Similar analysis for all measured samples results in a plot $E_f=E_f(n)$ which is shown in Fig. 4(b). Deviation of the experimental data points from the theoretical line is quite evident. Although at low concentrations (less than $1\times 10^{19}~{\rm cm}^{-3}$) 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 $1\times 10^{19}~{\rm cm}^{-3}$ one clearly observes a saturation of the Fermi energy. On the one hand, this result is surprising since it contradicts the standard theory. On the other hand, it could be expected since, as mentioned above, the electronic devices employing heavily doped InGaAs operated normally with no evidence of the Fermi energy spilling over the InAlAs barrier



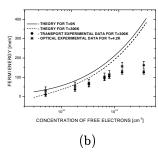


Figure 4: (a) Typical experimental I-V curve and its derivative for heterojunctions with Sn-doped semiconductors. The inset - vertical junction for I-V measurements and sample structure; (b) Experimental dependence of Fermi energy on carrier concentration in heavily doped InGaAs.

3 Conclusions

We have demonstrated that introduction of fixed charge into a heterostructure barrier significantly changes the I-V characteristics of thermionic diffusion, in such a way that the derivative curve exhibits a well-defined peak when the conduction band edges on both sides of the junction are aligned by the applied voltage. This situation can be successfully realized in experiment and used for determination of Fermi energy in semiconductors. Previously, only ballistic barriers were thought to possess a similar property, which was therefore difficult to employ in practice.

Using this novel transport technique, we have investigated the dependence of E_f on the mobile carrier concentration in heavily Sn doped InGaAs layers. 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's 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 free-electron estimates of the Fermi level exceeds 0.5 eV. When compared to the best available current theory the discrepancy is still as high as 0.25 eV. We believe our results are convincing enough to encourage the development a new theoretical model appropriate to heavily doped semiconductors.

Acknowledgments

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