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Photoreflectance study of photovoltage effects in GaAs diode structures

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Photoreflectance measurements of a GaAs p-i-n diode as a function of temperature (50–450 K) are reported. The photovoltage in the structure is obtained from the electric field strength which is determined from the Franz–Keldysh oscillations in the photoreflectance spectrum. The results are compared to those from an n-GaAs structure where the Fermi level is pinned at the surface. In this case the photovoltage can be determined only by fixing the energy of the Fermi pinning level. The theoretical photovoltages are also calculated from the ideal p-n and Schottky diode equations. This study clearly shows the importance of the photovoltage effects in the photoreflectance measurements.

The contactless modulation spectroscopy method of photoreflectance (PR) is frequently used to study the electronic energy levels in semiconductor microstructures. In PR the electron-hole pairs created by the pump light pulses are separated by the surface (or internal) electric field of the sample. Therefore, the electric-field strength is being modulated and PR is just a special case of electoreflectance. In addition to the electronic energy levels also the strength of the electric field can be determined from the PR spectrum if the material is of sufficient homogeneity for the Franz–Keldysh oscillations (FKO) to be observed on the high-energy side of the band gap energy. The method can be used to determine the surface electric field optically, and has been used to determine the position of the Fermi level on the surface of GaAs. However, the effect of the photovoltage on the electric field cannot be ignored in any spectroscopic method in which the sample is illuminated with photons with an energy larger than the band gap. In fact, the photovoltage has been shown to have a considerable effect in the soft x-ray photoemission measurements of GaAs. Also, the photovoltage caused by the pump and probe light in the PR measurement reduces the surface electric field. This effect can only be neglected at high temperatures (T > 400 K) or using very low light intensities.

The PR technique can also be used for probing the internal electric fields in semiconductor structures. The photovoltage can be expected to have a similar effect as in the surface electric-field measurement. In this work we report the optical determination of the photovoltage in a GaAs p-i-n diode. The results are compared with a surface-i-n (s-i-n) structure at temperatures between 50 and 450 K.

Two samples were grown on semi-insulating (100) GaAs substrates in a standard molecular beam epitaxy system using solid sources and Si and Be for the n- and p-type dopants, respectively. The layer thicknesses were calibrated using the reflection high-energy electron diffraction oscillation technique and x-ray diffraction measurements. The thicknesses of the intrinsic layers were also checked using C-V measurements. The p-i-n structure had a 4290-Å-thick undoped GaAs layer between two 1430-Å-thick n- and p-type GaAs layers. The free carrier concentration of both doped layers was about 10^{18} cm^{-3}. The s-i-n sample consisted of a 6500 Å n-type (n ≈ 10^{16} cm^{-3}) GaAs buffer layer, a 1300 Å n-type (n ≈ 10^{18} cm^{-3}) layer and a 2560 Å undoped surface layer.

The standard PR arrangement was used for the optical spectroscopy. The 488 nm line from an argon ion laser was used as the pump beam with a modulation frequency of 270 Hz. The intensity of the laser beam was attenuated to 1–10 mW/cm^2 with neutral density filters. The probe beam from a tungsten lamp passed through a 0.5 m monochromator with a typical resolution of 10–16 Å. A silicon photodiode was used for measuring the intensity of the reflected light. The sample was mounted in a closed cycle He cryostat capable of cooling down to 13 K.

The photovoltage at the surface, i.e., in the s-i-n structure, can be measured only by explicitly fixing the energy of the Fermi pinning level at the surface. However, in the p-i-n structure the position of the Fermi level in the p- and n-type materials is known (if the photovoltage effect is ignored). Therefore, the photovoltage, V_S, can be determined either by measuring the voltage between the n- and p-layers or by determining the electric field in the intrinsic layer. If the thickness, L, of the intrinsic layer is large compared to the thicknesses of the depletion layers the open-circuit photovoltage is simply

\[ V_S = \frac{E_g}{q} - FL, \]  

where \( E_g \) is the band gap. The electric field, \( F \), is determined from the extrema of the FKO, which are given by

\[ n \pi = \phi + \frac{4}{3} \left[ \frac{E_n - E_g}{\hbar \theta} \right]^{3/2}, \]  

where \( n \) is the index of the nth extremum, \( \phi \) is an arbitrary phase factor, and \( E_n \) is the energy of the nth extremum. The parameter \( \hbar \theta \) is

\[ \hbar \theta = \frac{\mu^2 F^2}{2\mu}, \]  

where \( \mu \) is the reduced effective mass for the electron and heavy-hole pair in the direction of the field. \( \hbar \theta \) is deter-
FIG. 1. Photoreflectance spectrum of the GaAs p-i-n sample at room temperature. The $E_0$ and $E_0 + \Delta_0$ transitions are shown. The Franz-Keldysh oscillation is seen on the high-energy side of the $E_0$ transition. The inset shows the sample structure.

mined from Eq. (2) by plotting the energy as a function of the extremum index:

$$E_n = \alpha \theta X_n + E_g$$

$$X_n = \left[ \frac{3\pi}{2} \left( n - \frac{1}{2} \right) \right]^{3/2}; \quad n = 1, 2, 3, \ldots$$  (4)

The intercept of the line and the $E_n$ axis yields the energy gap $E_g$.

A typical PR spectrum of the p-i-n sample at 290 K is shown in Fig. 1. The Franz-Keldysh oscillations are seen on the high energy side of the band edge ($E_0$) transition. As many as 15 extrema can be seen in the FKO due to the almost constant electric field. The weak $E_0 + \Delta_0$ transition can also be seen at the energy of 1.76 eV. A spectrum from the s-i-n sample recorded at 296 K is seen in Fig. 2. It closely resembles the spectrum obtained from the p-i-n sample. The amplitude of the FKO is remarkably reduced at the sixth extremum due to the interference between the oscillations from the heavy- and light-hole subbands. The insets in the figures give the structures of the samples.

FIG. 2. Room-temperature photoreflectance spectrum of the GaAs s-i-n sample. Similar features as in Fig. 1 can be seen. The inset shows the sample structure.

The electric fields in the intrinsic layers are determined from the measured FKO using $\mu = 0.055$ (in units of free-electron mass) for the reduced mass. As shown in Fig. 3, the electric-field strength is reduced at low temperatures due to the photovoltage. The photovoltage obtained from the PR measurements at different temperatures is shown in Fig. 4. The behavior of both diode structures is very similar. At high temperatures of 400–450 K the photovoltage disappears. As the temperature is lowered the photovoltage increases linearly towards a limiting value determined by the barrier height ($\eta V_F$ and $\eta E_g/\bar{q}$ for the s-i-n and p-i-n structures, respectively). The theoretical photovoltage for the s-i-n structure is calculated from the ideal Schottky diode equations Assuming the Fermi level to be pinned at 0.73 eV below the conduction band. The model provides a good fit to the experimental data when the photocurrent is $1 \times 10^{-11}$ A/cm$^2$ which is very close to the values (0.4–4 mA/cm$^2$) calculated from the pump-beam intensities. The results agree well with those by Yin et al. for a similar s-i-n

FIG. 3. Measured electric fields of the p-i-n and s-i-n samples as a function of the temperature. The photovoltage reduces the electric field strength at lower temperatures.

FIG. 4. Photovoltage of the p-i-n and s-i-n samples as a function of the temperature. The photovoltage approaches the limiting value of the barrier height as the temperature is lowered. The results from the s-i-n sample are fitted by using the ideal Schottky diode equations of Ref. 6 assuming $V_F = 0.73$ V and $J_{pc} = 1 \times 10^{-11}$ A/cm$^2$ (solid line). The data from the p-i-n sample is fitted by using Eqs. (5) and (6) assuming $J_{pc}/C = 1 \times 10^{-11}$ K$^{3/2}$ (dashed line). The ideality factor $\eta$ is 0.9 in both fits.
structure.\textsuperscript{6} An analogous calculation can be performed for the \textit{p-i-n} structure using the ideal \textit{p-n} diode equations,\textsuperscript{9} from which the photovoltage \( V_S \) is

\[ V_S = \frac{2\eta kT}{q} \ln \left[ \frac{J_{pe}}{J_S(T) + 1} \right], \tag{5} \]

in which \( J_{pe} \) is the photocurrent and \( \eta \) is the ideality factor. The saturation current \( J_S(T) \) is determined by the recombination current and its temperature dependence can be written\textsuperscript{9}

\[ J_S(T) = CT^{3/2} \exp \left( -\frac{E_g}{2kT} \right), \tag{6} \]

where \( C \) is a constant.

The main advantage of the \textit{p-i-n} structure compared with the \textit{s-i-n} structure is that the barrier height is well defined as the Fermi level position in the \textit{n}- and \textit{p}-type layers is known. Even though the ideal \textit{pn}-diode model resembles closely the model for the Schottky diode, the number of adjustable parameters is only two which is smaller than that of the Schottky diode model. By using values \( J_{pe}/C = 1 \times 10^{-4} \text{K}^{3/2} \) and \( \eta = 0.9 \) an excellent agreement between the experimental and theoretical results is obtained. From Eq. (6) the saturation current density at 300 K is 50 nA/cm\(^2\), which is of the same order of magnitude as in the \textit{s-i-n} structure. The value of \( C \) calculated from the recombination current model\textsuperscript{9} is approximately 1 A/cm\(^2\) K\(^{3/2}\), which is comparable to the experimental value of 8 A/cm\(^2\) K\(^{2}\).

In conclusion, we have compared the effect of the temperature on the photovoltage in GaAs \textit{p-i-n} and \textit{s-i-n} structures in the range from 50 to 450 K. We have found that both diodes behave in a very similar way. The determination of the photovoltage in the \textit{p-i-n} diode from the electric field strength in the intrinsic region does not require the knowledge of the surface Fermi energy pinning position. The results for both diode structures can be explained by the ideal diode equations.

\textsuperscript{1}See, for example, O. J. Glembocki, in \textit{Proceedings of the Society of Photo-optical Instrumental Engineers} (Society of Photo-optical Engineers, Bellingham, 1990), Vol. 1286, p. 2.


