Optical Absorption and Photoluminescence Measurements in InP and InP:Fe Bulk Crystals and Inspection of the Relations Between these Measurements

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Abstract

Optical absorption and photoluminescence (PL) measurements were carried out in both undoped and Fe-doped samples and the effect of Fe doping on absorption and PL spectra were studied. The results show that Fe or Fe-related defects behave as non-radiative recombination centers in InP. This is very important from the point of view that the control of minority carrier lifetime is possible. On the other hand, comparative analysis of the PL results with the optical absorption data show that quantitative assessment of relative PL intensities is possible with respect to Fe concentrations.

Key Words: InP, InP:Fe, photoluminescence, absorption, semi-insulating, band gap narrowing

1. Introduction

Semi-Insulating (SI) InP substrates are technologically becoming of great interest. Because they are key materials for high speed microelectronics and optoelectronic applications, the improvement of the quality of these substrates is important. Indeed this quality, in terms of device performance, is in a desired or undesired manner, strongly affected by deep levels which are first of all related to native defects or impurities in the starting material. Transition metals in III-V semiconductors, in particular iron (Fe), are often used as dopants in order to obtain InP single crystals with SI properties [1]. Due to the importance of SI materials in device fabrication and the availability of Fe doped

InP with very high resistivity form, the properties of Fe and related defects in InP have been widely investigated [2].

Undoped InP grown by Liquid Encapsulated Czochralski (LEC) process and some other bulk growth techniques comes out as n-type because of unintentionally contaminated shallow donors. Fe doping results in a compensation of these donors by the Fe acceptors substituting for indium (In) situated near the midgap level leading to highly resistive SI material. As there is a direct correlation between substrate properties and device characteristics, the characterization of these Fe or Fe-related defects is of great importance in order to produce good quality devices [3].

In this study, we have performed a set of parallel optical absorption and photoluminescence measurements in InP and InP:Fe materials. We obtained reverse correlation between quantum efficiency and Fe concentration. We show that optical absorption measurements provide direct quantitative estimation of Fe concentrations in InP.

2. Experimental

In order to observe the effects of Fe doping in InP crystal, two identical 5 cm diameter wafers (InP and InP:Fe) grown by LEC technique under exactly the same thermal conditions. From each wafer 8 samples of about $3x2 \text{ mm}^2$ were cut off from the center up to the edge and investigated. The thickness of both wafers is the same at about 370 μ m. Parallel optical absorption and PL measurements were performed on both undoped and Fe doped samples for a healthy comparison of data.

Optical absorption measurements were performed with a near IR spectrometer. The wavelength resolution of the spectrometer is 3 nm. The samples had had commercial polishing treatments before we cleaned with the ultrasonic baths of trichlorethylen, acetone and methanol, respectively.

PL experiments were performed with a conventional PL kit using lock-in technique. A 300 mW (maximum power) Ar-ion laser was used to produce electron-hole pairs. A closed cycled He cryostat was used to vary the temperature from 10 K to 300 K. A Ge detector kept at a constant temperature of 77 K was used to detect the luminescence emitted from samples. A 50 cm spectrometer with a wavelength resolution of better than 2 nm was used for dispersive analysis of the luminescence.

3. Results and Discussions

Fornari and Kumar have shown that overall intra-bandgap absorption made by the Fe atoms situated close to the middle of the energy gap of InP crystals increases in Fe doped samples [4]. They have calibrated this absorption at a wavelength of 1000 nm with respect to the Fe concentrations. According to the calibration derived by Fornari and Kumar, an absorption coefficient of 1 cm^{-1} at a wavelength of 1000 nm corresponds to Fe concentration of 7.7 x10¹⁶ cm⁻³. This provides a non-destructive quantitative technique to measure Fe concentration in SI InP.

We also show that Fe doped samples exhibit higher intra-bandgap absorption than that of undoped samples, as seen in Figure 1. To convert the absorbance data to absorption coefficient values, we made use of equations which were previously proposed for normal incidence of light on Fe doped InP [4] and gallium arsenide [5].



Figure 1. Optical absorption spectra of undoped and Fe doped InP.

$$R = \frac{(n-1)^2}{(n+1)^2} \tag{1}$$

$$T = \frac{(1-R)^2 \exp(-\alpha t)}{1-R^2 \exp(-2\alpha t)},$$
(2)

where R, T and A are the reflectivity, transmittance and absorbance, respectively; n is the refractive index, α the absorption coefficient and t the sample thickness. We assume that in undoped samples the optical absorption due to Fe should be zero at all intra-bandgap wavelengths. Therefore Eq. (2) reduces to

$$T = \frac{(1-R)^2}{1-R^2} = \exp(-A) \tag{3}$$

over the entire intra-bandgap wavelength range in an undoped material. From this equation we determine the reflectivity R. Having determined R, we can easily calculate α values for each Fe doped samples. From α values at 1000 nm wavelength, we can determine Fe concentration of the samples, using the calibration of Fornari and Kumar [4].

From α^2 versus photon energy plots near the bandedge tail, we determine the bandgaps of all the samples by extrapolation of α^2 values to zero. We show that bandgap narrowing occurs due to Fe doping. The shrinkage of the bandgap is proportional to

[Fe]^{1/2}, as seen in Figure 2. This is quite consistent with the theory predicted by Hrivnak [6].



Figure 2. Bandgap narrowing due to Fe doping, in agreement with the theory predicted by Hrivnak [6].

As seen in Figure 3, there are three peaks observed in the near bandedge of undoped and Fe doped InP samples. The peaks at 1.415 eV energy at sample temperature of 10 K is exciton decay at neutral shallow donors [7]. The peak at 1.377 eV is a shallow donor-shallow acceptor pair transition and the peak at 1.334 eV is phonon replicas of the 1.377 eV peak [8].



Figure 3. Near band edge photoluminescence spectra of undoped and Fe doped InP at sample temperature of 10 K.

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Overall near bandedge luminescence is reduced more than 98% and 70%, respectively, at 1.377 eV and 1.415 eV peaks in all the Fe doped samples as shown in Figure 4. It follows that PL intensities in Fe doped samples are anti-proportional to the Fe concentrations. This is due to the fact that Fe atoms behaves as non-radiative recombination centers in SI InP, as discussed earlier [9]. In general, as the concentration of Fe determined by optical absorption measurements increases, reduction in near bandedge PL intensities at peak values increases and saturates to a value almost 99.8% at concentrations higher than 9×10^{16} cm⁻³ (Figure 4). This implies that the near bandedge PL mapping of wafers can not distinguish the variations in regions with Fe concentrations higher than 9×10^{16} cm⁻³. Although this is high Fe concentrations in commercially available samples, this result show that optical absorption is necessary in samples with Fe concentrations higher than 9×10^{16} cm⁻³ for qualification of InP substrates. On the other hand, Figure 4 provides quantitative assessment of relative PL intensities with respect to Fe concentrations.



Figure 4. Reduction in near band edge PL intensities as a function of Fe concentrations in InP for 1.377 eV and 1.415 eV peak.

4. Conclusions

We demonstrate that optical absorption technique provides quantitative measurements of Fe concentrations in SI InP. Near bandedge PL measurements show that the intensities are reduced more than 98% and 70%, respectively, at 1.377 eV and 1.415 eV peak energies, the precise value depending on Fe concentration in the material, indicating that quantitative assessment of relative PL intensities is possible with respect to Fe concentrations. Relative near bandedge PL intensities is anti-proportional to Fe concentration, proving that Fe or related defects play a role as non-radiative recombination center in SI InP.

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