# A-3-4 A New Method of Characterizing the In-depth Profile of Thermally Induced Defects in CZ Si

Hiroshi NAKAYAMA, Johji KATSURA, Taneo NISHINO and Yoshihiro HAMAKAWA

Faculty of Engineering Science, Osaka University

Toyonaka, Osaka 560.

We propose a new photoluminescence(PL) method to characterize quantitatively the in-depth profile of thermally induced defects in CZ-Si. This method is based on the theoretical considerations on the recombination kinetics of the free exciton(FE) and trapped exciton(TE) system at 4.2K and free carrier(FC) and trapped carrier(TC) system at 300K, taking into account the diffusion phenomena of photoexcited FE and FC. In the present work, this PL technique has been applied to the characterization of thermal-oxidation induced surface and bulk defects, the results suggesting that this PL method is also useful for the intrinsic-gettering technique currently used in VLSI technology.

## Theoretical Considerations

Recently, based on a model for the exciton-recombination kinetics, we have succeeded in explaining quantitatively the photoexcitation-power and dopant-content dependences of the exciton-PL intensity at 4.2 K in impurity-doped Si[1]. The analysis method has been applied to the content determination of a small amount of dopant impurity involved nearly homogeneously[2]. However, it often becomes more necessary to characterize the density of grown-in or process-induced defects distributing rather heterogeneously in the crystal as in the case of thermally induced defects caused by oxygen precipitation in CZ-Si. For this purpose, the above-mentioned formula has been generalized to include the TE and TC states associated with such thermal defects and further effects of the diffusion phenomena of photoexcited FE and FC.

Using the usual boundary conditions; $D\frac{dN(z)}{dz}=SN(z)$ at $z=0$ and $N(\infty)=0$, the solution of the well-known one-dimensional diffusion equation which is applicable to both FE and FC is described as[3)]

$$N(z)=\frac{G(0)L^2}{D}(1-\alpha^2L^2)^{-1}\left[\exp(-\alpha z)-\frac{\alpha+S/D}{1/L+S/D}\exp(-z/L)\right], \quad (1)$$

where $N(z)$ denotes the density of FE or excess FC(minority carrier), $G(0)$ is the FE (or FC) generation rate at $z=0$ and $z$ is the normal distance from the surface. Typical calculated results of the depth profiles of photoexcited FE (at 4.2K) and FC (at 300K), using the parameters in Table I, are shown in Fig.1, in the case of Si:B ($N_B=10^{15}$cm$^{-3}$) under the photoexcitation of 4 Wcm$^{-2}$ at 5145 Å by a cw Ar$^+$ laser. As can be seen in the figure, the density profiles of FE and FC strongly depend on their corresponding diffusion length L. Here, we can write the diffusion length, considering the recombination kinetics of the FE-TE and FC-TC system as

$$L_X=[D_X/(W_X+C_{0,B}N_B+C_{0,T}N_{T,X})]^{1/2} \text{ for FE, } L_n=[D_n/(W_Pp_0+C_{T,n}N_{T,n})]^{1/2} \text{ for EC.} \quad (2)$$

Here, $N_{T,X}(N_{T,n})$ is the density of thermally induced exciton(electron) traps and $C_{T,X}(C_{T,n})$ denotes the corresponding exciton(electron)-capture rate. Integrating the desity of FE or FC in the z-direction, we obtain approximately these trap densities as a function of PL-intensity reduction rate. That is,

$$N_{T,X}\simeq[(W_X+C_{0,B}N_B)/C_{0,T}][(I_X^0/I_X)-1],\ N_{T,n}\simeq(W_PN_B/C_{T,n})[(I_{BB}^0/I_{BB})-1], \quad (3)$$

where $W_X(W_p)$ is the intrinsic recombination rate of FE(electron-hole pair) and $I_X^0(I_{BB}^0)$ and $I_X(I_{BB})$ are FE(band-to-band) PL intensities before annealing and after annealing, respectively. From Eq.(3), we can estimate the densities of themally induced defects having the nature of an exciton trap by PL measurements at 4.2 K and also those having the nature of a carrier-trapping and/or recombination center by room temperature (at 300K) PL measurements.

Application to the Characterization of Thermal-Oxidation Induced Defects

The PL method mentioned above has been utilized to characterize the thermal-oxidation induced defects in CZ-Si wafers. The samples used here were two kinds of CZ Si:B having the oxygen content, before oxidation, of $10.3\times10^{17}cm^{-3}$(high oxygen CZ-Si) and $7.4\times10^{17}cm^{-3}$(low oxygen CZ-Si). Thermal oxidation was performed for 16 hours at 1000 °C in wet oxygen ambient. Room temperature PL measurements were carried out on the bare surface of the oxidized wafer whose thermally grown oxide layer was removed by chemical etching to observe the surface defects. So as to characterize the bulk defects, PL spectra were also taken on the etched surface of the wafer whose 50 μm Si-layer was removed further. Figure 2 shows the room temperature PL spectra due to band-to-band recombination taken from the surface and the bulk, namely in the depth of 50 μm, of the oxidized wafer, comparing with that of as-received wafer. As can be seen from the figure, the PL intensity drastically decreases with thermal oxidation, and also the reduction rate in relation to as-received wafer is larger for the bulk than for the surface (See the insert of Fig.2). Hence, from the simple analysis of such PL-intensity reduction, we can estimate the density of the generated defects on the basis of Eq.(3) for both the surface and the bulk. As a result, it has been found by the PL technique that the density of the bulk type defects induced by thermal oxidation at 1000 °C is higher than that of the surface type defects, and also the defects densities are higher for high-oxygen Si wafers than for low-oxygen wafers. This results well correspond to the optical micrographic observation using Dash etching performed on these samples.

References


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Table I. Parameters for the calculation of depth profiles of FE and FC

| | FE(4.2 K) | FC(300 K) |
|---|---|---|
| D, $cm^2s^{-1}$ | 150 | 30 |
| S, $cm\ s^{-1}$ | 0 | $10^3$ |
| $\alpha$(5145 Å), $cm^{-1}$ | $10^4$ | $10^4$ |

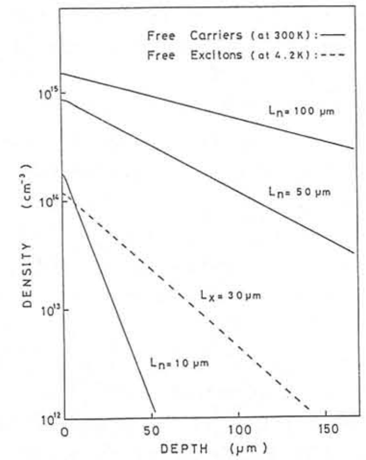


Fig. 1. Theoretically calculated depth profiles of photoexcited FE and FC.

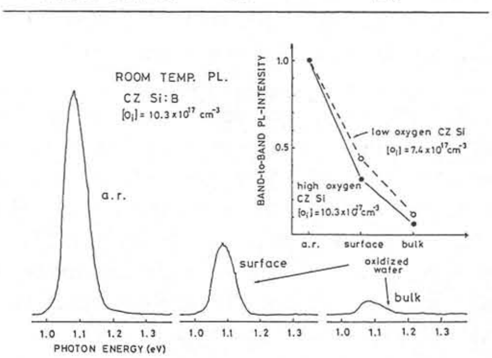


Fig. 2. Room temperature PL of surface and bulk of thermally oxidized wafers.