JOURNAL OF MATERIALS SCIENCE 25 (1990) 4298–4300

X-ray double-crystal diffractometry characterization of semi-insulating GaAs

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The X-ray double crystal diffractometry method was employed to measure variations in dislocation densities, and normal residual strains in undoped, and indium-doped semi-insulating GaAS wafers grown by the liquid-encapsulated Czochralski technique. Low thermal gradient growth conditions, and indium doping decreased dislocation densities significantly. The distribution of dislocation densities was similar to the variation in EL2 concentrations. Normal residual strains were high in the undoped sample grown under the high thermal gradient growth conditions. The strain values were considerably lower in the undoped sample grown under the low thermal gradient growth conditions. Indium doping increased the strain slightly.

1. Introduction

Semi-insulating GaAs wafers are currently being used in the development of a number of high-performance electronic devices. These include low- and high-power field effect transistors, monolithic microwave integrated circuits, high-speed digital integrated circuits, and high-speed charge-coupled devices. The high resistivity of this material is due to an electrical compensation resulting in the Fermi level being pinned to a midgap deep-level donor labelled EL2. Therefore, the uniformity of the semi-insulating property, which is highly desirable, depends on the uniformity of the distribution of EL2 concentrations.

The liquid-encapsulated Czochralski technique is mostly used to grow these GaAs (0 0 1) single crystals. It has been reported that the distribution of EL2 concentrations across the diameter of the crystal (i.e. [1 1 0] direction) follow a "W" pattern [1, 2]. Also, a strong similarity has been found between the patterns of EL2 concentrations, and dislocation densities [1, 3, 4]. Dislocation densities were measured by the etch-pit density method.

The X-ray double-crystal diffractometry technique offers an excellent possibility to measure dislocation densities, and overall strains in GaAs crystals. This method is non-destructive and can be rapidly performed. In this paper, distributions of dislocation densities and residual strains in undoped and indium-doped semi-insulating GaAs, as determined by the X-ray double-crystal diffractometry method, is reported. Dislocation density profiles were also compared with variations in EL2 concentrations.

2. Experimental procedure

GaAs wafers of 75 mm diameter were obtained from Rockwell International, Thousand Oaks, California. Three different samples were used; two samples were undoped, and one sample was indium-doped with a doping concentration of 0.18 at.%. Also, one of the undoped samples was grown under high thermal gradient growth conditions, while the other undoped sample and the indium-doped sample were grown under low thermal gradient growth conditions [5]. X-ray rocking curves were measured using a Blake Industries double-crystal diffractometer in (+/−) arrangement [6] and Cu$K\alpha_1$ radiation. A perfect crystal of germanium (0 0 1) was used as the first crystal. Rocking curves of the (0 0 4) reflection were obtained in 5 mm steps in the middle part of the crystal across the [1 1 0] direction.

X-ray Berg–Barrett topographs of wafers were taken using a Lang camera and Cu$K\alpha_1$ radiation [7]. The (2 2 4) reflection was used in this case, and because the largest size of the topograph was limited to 1 cm long and 2 cm wide, the X-ray topograph of the middle portion of the wafer was taken in four different sections.

3. Results and discussion

Deconvoluted [8] values of full-width at half-maximum (FWHM) of the (0 0 4) rocking curves are shown in Fig. 1 (FWHM of a perfect germanium crystal for the (0 0 4) reflection was found to be 5.7 arc sec). The dislocation density can be calculated from the FWHM, β, as follows

$$\beta_{\text{deconv.}} = \frac{\beta_{\text{meas.}}}{1.4} \quad (1)$$

The dislocation density, D, is then given as [9]

$$D = \frac{\beta_{\text{deconv.}^2} - \beta_{\text{perfect}^2}}{9.0\, \boldsymbol{b}^2} \quad (2)$$

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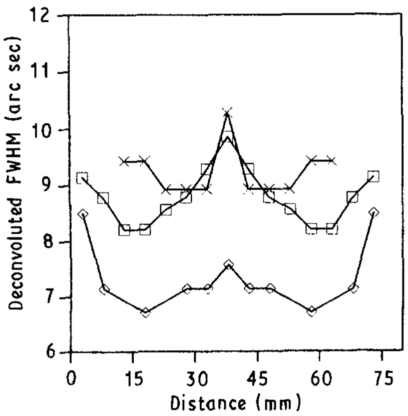

Figure 1 Variations of FWHM across the diameter of the wafers. (x) High gradient, undoped; (□) low gradient, undoped; (◇) low gradient, indium-doped.

where β_{perfect} is calculated from Darwin's theory [8], and it is assumed that perfect crystal does not contain any dislocations. The value of β_{perfect} of GaAs (0 0 4) is 5.6 arc sec, while that of germanium (0 0 4) is 5.7 arc sec. $\boldsymbol{b}$ is the Bergers vector in the [0 1 1] direction, and it is equal to 0.2448 nm.

Dislocation densities, as calculated, are plotted in Fig. 2. Dislocation density distributions across all the wafers have "W" shapes indicating symmetry. Dislocation densities in the crystal grown under the low thermal gradient growth conditions were lower compared to those in the crystal grown under high thermal gradient growth conditions. Indium doping of the wafer under the low thermal gradient growth conditions reduced dislocation densities further. Considerable reduction of dislocation density has, also, been reported previously [5, 10]. This is due to the suppression of nucleation and propagation of dislocations by solid solution hardening mechanism. The dislocation density values obtained by the X-ray method are comparable to those obtained by the etch-pit density technique [5].

From the shift of the rocking curve peak-position of the (0 0 4) reflection, $\Delta\Theta$, the normal residual strain, ε, can be calculated using the Bragg diffraction condition

$$\varepsilon = \frac{\Delta d}{d} = -\cot \Theta \, \Delta\Theta \qquad (3)$$

where d is the interplanar spacing, Δd is the change in interplanar spacing and Θ is the Bragg angle. Fig. 3

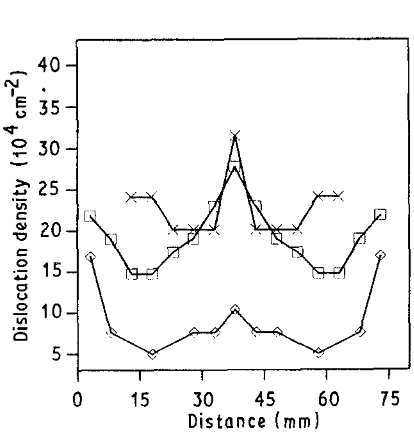

Figure 2 Dislocation density profiles across the diameter of the wafers. For key, see Fig. 1.

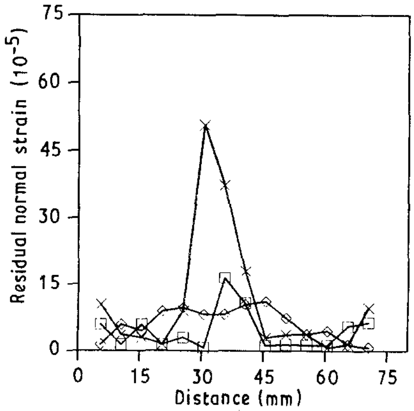

Figure 3 Variations of residual strains across the diameter of the wafers. For key, see Fig. 1.

shows the variation of normal strain values with the distance across the wafers. It can be seen that strains are high in the middle part of the wafer grown under high thermal gradient growth conditions. Low thermal gradient growth conditions decreased the strain considerably. The strain values increased only by a small amount by indium doping. The X-ray Berg–Barrett topography of the wafer grown under high thermal gradient growth conditions, as shown in Fig. 4, indicates a large strain present in the middle part of the sample. In order to take a topograph of that region, the traverse had to be limited to 6 mm, and even then, the whole portion of the crystal did not come into reflection.

EL2 concentration profiles, as plotted in Fig. 5, show a symmetry for all the wafers. An optical absorption method was used to measure the EL2 concentration [3]. The EL2 concentration values were found to be lowest and rather uniform in the indium-doped wafer, intermediate in the undoped wafer grown under the low thermal gradient configuration, and highest in the undoped wafer grown under the high thermal gradient configuration. Comparing Figs 2 and 5, it can be observed that there are some similarities between the dislocation density and EL2 concentration distributions.

4. Conclusions

It was demonstrated that the X-ray double crystal diffractometry can be used successfully to measure the variation in dislocation density and overall strain in semi-insulating GaAs wafers. This non-destructive method does not need any sample preparation, and has a short data acquisition time. It was further shown

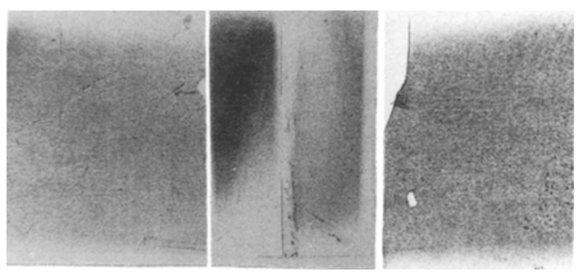

Figure 4 The X-ray Berg–Barrett topography of the undoped GaAs wafer grown under the high thermal gradient growth conditions (Cu$K\alpha_1$ radiation, (2 2 4) reflection, magnification 2x).

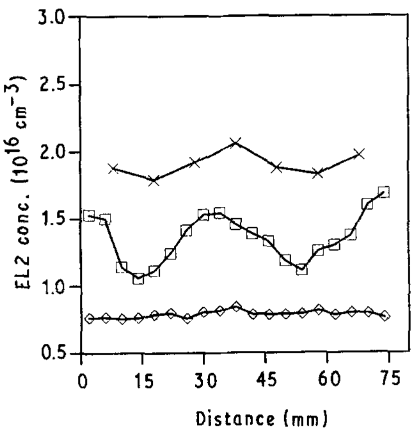

Figure 5 EL2 concentration profiles across the diameter of the wafers. For key, see Fig. 1.

that low dislocation densities were achieved by the low thermal gradient configuration and indium doping. Residual strains decreased considerably using the low thermal gradient growth conditions even for indium doping, which increased the strain by a small amount. Good correlation was obtained between the EL2 concentration and dislocation density profiles for the undoped wafers. The variation in EL2 concentrations in the indium-doped samples was found to be small.

Acknowledgement
This work was funded in part by the National Science Foundation Grant no. DMR-8 605 564.

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Received 25 May
and accepted 23 October 1989