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EFFECT OF DOPING ON $Ga_{1-x}Al_xAs$ STRUCTURAL PROPERTIES

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The microstructure of $Ga_{1-x}Al_xAs$ layers was studied using methods of high resolution diffractometry and topography. Mapping out the reciprocal space in the vicinity of 004 reciprocal lattice points shows a difference in diffuse scattering between doped and undoped layers. This result is attributed to a difference in a point-defect density. From the measurements of lattice parameters at different temperature it was found that the thermal expansion coefficients for the doped layers are higher than for the undoped ones. This phenomenon is attributed to the change of the anharmonic part of lattice vibrations by free electrons or/and point defects.

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1. Introduction

Doping of semiconducting-materials influences their structural properties, for example, their lattice parameters and microstructure. Dislocation loops, as well as clusters of intrinsic point defects, which are not visible on topographs, can be revealed and investigated by X-ray diffuse scattering, even in the case where defects are not visible in a transmission electron microscopy [1]. Lattice parameter measurements with an accuracy of 10^{-5} Å are sensitive to point defects and their distribution in the crystal lattice. For pseudobinary semiconductors, such

as $Ga_{1-x}Al_xAs$, the effect of doping on lattice parameters is extremely difficult to determine, because of a concurrent strong effect of Al substitution. The typically used techniques (luminescence, X-ray microprobe, secondary ion spectroscopy) allow us to determine the x value within an accuracy of approximately $\Delta x = 0.01$. Such accuracy corresponds to $\Delta a = 0.00007$ Å, which is comparable to the effect of a typical dopant concentration. The problem mentioned above may be overcome by using temperature as an additional parameter.

In the present work, the layers of $Al_xGa_{1-x}As$ were characterized using X-ray diffuse scattering, X-ray topography, dislocations density and precise lattice parameters measurements. These methods were applied to gain a better understanding of crystallographic structure changes of doped AlGaAs layers.

2. Experimental

The 3 μm AlGaAs:Te layers were grown by liquid phase epitaxy (LPE) and 2 μm AlGaAs:Si layers and superlattice were grown by molecular beam epitaxy (MBE) on (001) oriented semiinsulating GaAs substrates. Undoped and Si doped superlattices GaAs/$Al_{30}Ga_{70}As$ (doped GaAs and AlGaAs) consisting of 120 periods of 20 monolayers GaAs/20 monolayers AlGaAs were deposited on 1 μm GaAs buffer layers.

Electric transport parameters for layers were determined from the Hall effect and an electron concentration, for all samples, was approximately $2\text{–}3 \times 10^{18}$ cm^{-3}. For the AlGaAs:Te layers this value was practically equal to the dopant concentration, but for the Si doped superlattices, the dopant concentration was higher (10^{19} cm^{-3}) due to the compensation effect. The Al concentration was determined in two ways: by microprobe and the precise lattice parameters from measurements of 006, 335 and 117 reflections (the Bond method). The lattice parameters were determined in a double-crystal configuration (for high temperatures from 300 K to 673 K) and also by using the high resolution Philips material research diffractometer (MRD) in a triple crystal configuration (at room temperature).

Using 004 Bragg reflection, reciprocal space maps for all samples were obtained in order to study diffuse scattering. Density of dislocations was calculated from the measurements of several (hkl) rocking curve widths [2]. When the broadening due to curvature and crystals size is negligible (i.e. layers thicker than 1 μm are deposited on substrates at least one hundred times thicker) dislocations cause broadening of the rocking curves in two ways:

(i) introducing a rotation of the crystals lattice;

(ii) introducing strain field surrounding the dislocations.

The measured rocking curve width (FWHM) for hkl reflection is given [2] by the following formula:

$$\beta_m^2(hkl) - \beta_o^2(hkl) - \beta_d^2(hkl) = \beta_{\text{adj}}^2 = K_\alpha + K_\varepsilon x \tan\Theta,$$

where β_m is the measured rocking curve width, β_o is the intrinsic rocking curve width for the crystal being examined, β_d is the intrinsic rocking curve width of the Bartels monochromator, β_{adj} is the rocking curve width adjusted to account for the intrinsic rocking curve widths, K_α and K_ε are angular and strain broadening, respectively. Then the dislocation density, D, may be determined independently

from K_α and K_ε as follows:

$$D = K_\alpha/4.3b^2,$$

$$D = K_\varepsilon/(0.0909b^2|\ln(2\times10^{-7}\mathrm{cm}\sqrt{D})|).$$

In this paper, FWHM for 004, 006, 335, 115 and 711 reflections of substrates and layers were measured. The Burgers vector b was taken equal to $a\sqrt{2}[110]$, where a is the lattice parameter.

Synchrotron X-ray topography is a method to study crystalline defects in semiconductors [3, 4]. Depending on the method used, topography may be sensitive to very small strains or strain gradients inside the crystal. For high photon energies the kinematical image of the deformation field caused by defects becomes wide making the detection of small defects easier. This is due to the fact that the intrinsic diffraction width of the dynamical crystal reflection decreases when photon wavelength decreases.

The X-ray synchrotron topography was made at D5 optics beam line at the European synchrotron radiation facility (ESRF). The radiation source of this beam line is a bending magnet with a usable photon spectrum of 6–80 keV. The reflections were recorded on a Kodak So-343 high resolution film with a resolution of about 1 μm. During the measurement the distance between sample and film was of the order of 25 cm, leading to a geometrical resolution of approximately 1 μm. The doped and undoped layers were measured in transmission (Laue) geometry. White beam topography was employed for a quick verification of the quality of the samples.

3. Results

The in-plane lattice parameters, of all investigated layers and superlattice were found equal to the lattice parameters of the substrates over the whole temperature range, the lattice parameters and thermal expansion coefficients in the growth direction differ drastically from their bulk value. The relaxed lattice parameters and thermal expansion were evaluated taking into account a linear relation between the Poisson ratios, ν, of GaAs and AlAs [5]. The thermal expansion for the doped and undoped relaxed $Al_xGa_{1-x}As$ layers in the whole range of x is given in Fig. 1. It can be seen that for the doped samples the thermal expansion is higher than for the undoped ones. The thermal expansion of the layers was found equal to the thermal expansion of the superlattice with the same mean $\langle x\rangle$ value as in the layers. The mean Al content $\langle x\rangle$ is related to Al content x in pseudobinary compound by the expression, $\langle x\rangle = x(n_1/n_1+n_2)$, where n_1 and n_2 are the numbers of GaAs and $Al_xGa_{1-x}As$ monolayers, respectively, in the superlattice unit cell.

The density of dislocations calculated for the substrate and layers/superlattice was found to be the same as for the substrate and equalled about 10^5 cm^{-2}.

Figure 2 shows 004 reciprocal-space scans of undoped (Fig. 2a) and doped (Fig. 2b) layers. An increase in diffuse scattering is easily observed for the doped samples. Due to the same dislocation concentrations of the doped and undoped layers diffuse scattering is caused by point defects or their agglomerates.

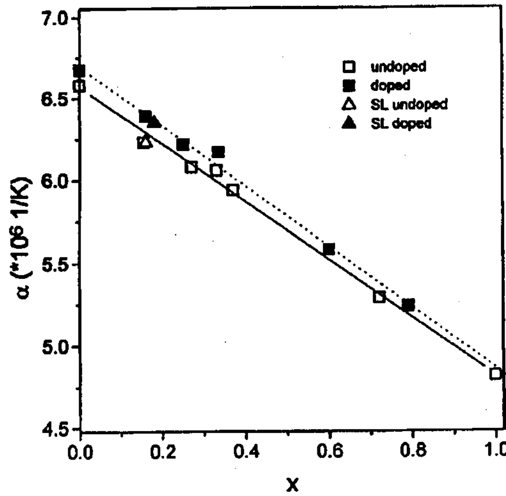

Fig. 1. Thermal expansion coefficient of undoped and doped AlGaAs layers and superlattice.

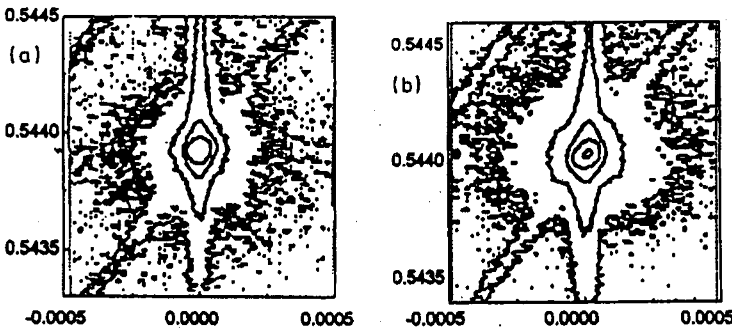

Fig. 2. Reciprocal space maps around 004 reciprocal space point for: (a) undoped layer, (b) doped layer. The axes are marked in units $\lambda/2d$.

There are no major differences between topographs of doped and undoped samples. In both topographs a contrast of the complex defect structure is observed.

4. Discussion

An increase in diffuse scattering observed for the doped $Al_xGa_{1-x}As$ layers is caused probably by point defects or their agglomerates [1], which are too small to be observed on topographs. The thermal expansion is related to the existence of anharmonic contribution in the interatomic potential. The shape of the interatomic potential which can be modified by point defects [6] or the phonon–electron interactions [5] influences the thermal expansion. Doping of $Al_xGa_{1-x}As$ layers introduced simultaneously point defects, their agglomerates and free electrons. Generally, it is difficult to distinguish the effects caused by the above-mentioned

factors. However, some conclusions may be drawn by comparing results for variously doped samples. For example, for the low temperature (LT) grown GaAs layers with a very high over-stoichiometric arsenic concentration, it was observed [7] that the thermal expansion is smaller with respect to stoichiometric semiinsulating (SI) GaAs. The LT GaAs layers possess arsenic precipitates and the lattice constant similar to GaAs:Te (bigger than for SI GaAs), but they have a very small free-electron concentration. For our doped $Al_xGa_{1-x}As$ layers we observed a bigger thermal expansion what suggests that this increase in thermal expansion coefficient is rather caused by free electrons. This conclusion is in agreement with the works of Kontorova [8], Zhdanova [9], Zhdanova and Kontorova [10], who found an increase in thermal expansion for n- and p-type germanium and correlated it with the electronic effect on the elastic constants. However, further research is necessary to clarify this point.

An influence of the elastic interaction through the interface on the thermal expansion of the superlattice is not detected. It is interesting that the thermal expansion, which essentially depends on the real structure, especially on the strain state of the lattice, is not changed by the strain existing in the superlattice. This effect was also observed by Clec'h et al. [11] for GaAs/AlGaAs superlattice for which the thermal expansion at low temperatures was measured.

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