Contemporary heterostructures for solar cells improvement

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Abstract. Current investigation is focused on InₓGa₁₋ₓP and InₓAl₁₋ₓP epitaxial layers growth. Multicomponent nanoheterostructures are the main materials for a contemporary triple-cascade solar cell, and for perspective photovoltaic devices. The optimal InₓGa₁₋ₓP and InₓAl₁₋ₓP growth process characteristics are determined. InₓGa₁₋ₓP epitaxial layers (with In & Ga varied on Ge), and InₓAl₁₋ₓP layers (with Al & In varied on Ge and GaAs) are investigated. During investigation X-ray diffractometry was used. Based on results of X-ray diffractometry the lattice parameter and In / Ga / Al ratio in the structure were detected. Solid phase versus the gas phase composition correlation was found based on the lattice parameters. It is determined that diffraction X-ray peaks broadening can be used as a parameter for the heterostructure perfection analyze. For the InₓGa₁₋ₓP solid solution (X = 45–53 %) and for InₓAl₁₋ₓP solid solution (X = 46–51 %) a high quality of the single-crystal structure and a slight diffraction X-ray peaks broadening are detected.

1. Introduction

Modern solar cells (SC) for satellites and spacecrafts are AⅢBⅤ cascade solar cells. A contemporary multi-cascade solar cell is a high technology item. SC multicomponent nanoheterostructure contains more than thirty InGaP / InGaAs / Ge layers which are grown by metalorganic chemical vapour deposition (MOCVD). To reach the high parameters it is need to correspond the requirements for the properties uniformity in films [1-3].

To detect defects nature, it is important to find the correlation between the structure and the MOCVD properties. The lattice parameters correspondence in the layers is very important. For the AₓB₁₋ₓC films growth it is useful to understand the correlation of the solid phase composition versus the third group elements ratio A / (A + B) elements in the vapour phase flow for growth conditions. The current investigation is for the InₓGa₁₋ₓP and InₓAl₁₋ₓP materials analyze.

2. Experiment

Samples of multicomponent nanoheterostructures were grown for the current investigation: InₓGa₁₋ₓP nanoheterostructures with In & Ga concentration in the range X = 38-53 %, doped by Si or Te on Ge; at the same time samples of InₓAl₁₋ₓP nanoheterostructures with In & Al concentration in the range X = 46-51 % on the Ge and GaAs were prepared, too. MOCVD method was used in our investigation for samples growth.
For epitaxial layer growth with specify properties (the lattice constant or the forbidden band) it is important to create specific crystal lattice in layers of heterostructure. In turn, for the applied constructions of alkyl sources (bubblers), the mole flow rate (the source stream concentration) at the bubbler output can be corrected [3-8]. In figure 1 investigated structure layers are presented.

Figure 1. Sample structures scheme: a – with In$_x$Ga$_{1-x}$P layer, b - with In$_x$Al$_{1-x}$P layer.

X-ray diffractometry (XRD), based on a two-crystal Vector diffractometer is used to determine the lattice constants for each layer by the rocking curves analysis. In our experiment the main impact to the intensity was given by thickest layer in the heterostructure (Ge substrate). The broadening and some other separately standing peaks shows layers presence that are mismatched by lattice parameters. As a peak with a reduced intensity is situated at the left side of the main one, the layer lattice constant increases according to the substrate, with a location at the right side - decreases. To calculate the In / (In + Ga) ratio of the In$_x$Ga$_{1-x}$P epitaxial layer in the solid phase, it is necessary to measure the distance between peaks equal to $d_{2\theta}$. Based on the lattice constant and the interplanar distance for a cubic cell correlation which is presented by Eq. (1), as well as by the Wolf-Bragg formula, it can be calculated the lattice constants. So according to Vegard law (2), it is possible to determine the epitaxial layer chemical composition:

\[ a^2 = \frac{d^2}{n}(H^2 + K^2 + L^2) \]  

(1)

where $a$ – lattice constant (nm), $d$ – interplaner distance between reflecting planes (nm), $n$ – diffraction reflection coefficient, $H$, $K$, $L$ – interference coefficient.

\[ a_{In_xGa_{1-x}P} = x \cdot a_{InP} + (1-x) \cdot a_{GaP} \]  

(2)

where $X$ – In content in solid solution.

3. Result and Discussion

The measured results correlate with liner dependence according to the Vegard law. At the same time in the Ge lattice parameter area there is not standard situation. The rocking curves at grown heterostructure were controlled by peak broadening (800 arc seconds) (figures 2a, 2b). At structure without defects distance between rocking curve peaks commonly is 200 - 400 a. u. and the broadening –not less than 200 (figure 2b). The In$_x$Ga$_{1-x}$P lattice parameter vs the In / (In + Ga) ratio in the vapour phase dependence based on the XRD results is shown in figure 2c. In$_x$Ga$_{1-x}$P lattice constants rises at In concentration growth. The lattice parameter mismatch is 0.1 - 0.26 %. After the samples measurements it was detected that at In concentration in the range 45 - 53 % the single-crystal multicomponent nanoheterostructure was good quality. Using In& Ga ratio (1:1), such film performed the best properties with lattice constant close to the Ge. The composition range in samples was – 0.5 – 3 %. Investigations to determine the solid solution composition homogeneity over the entire surface of the sample were carried out. Oscillation curves were measured along the sample radius (coinciding with the growth chamber radius). It was detected that the lattice constants mismatch is not more than 0.1 % (the values scatter does not exceed 6 %). Such result proofs proper measuring at
the central point of the sample area. $\text{In}_{x}\text{Al}_{1-x}\text{P}$ epitaxial layers on Ge & GaAs were checked similarly. It was detected correlation between nanoheterostructure lattice constants and a linear dependence according to the Vegard law in the range $X = 46 - 53\%$ (figure 3).

**Figure 2.** Dependence of the $\text{In}_{x}\text{Ga}_{1-x}\text{P}$ lattice constant: a, b - rocking curves for different $\text{In} / (\text{In} + \text{Ga})$ ratios in the solid phase (a - sharp peak, b - two spaced peaks overlap), c - the dependence of the epitaxial layers $\text{In}_{x}\text{Ga}_{1-x}\text{P}$ lattice constant vs the $\text{In} / (\text{In} + \text{Ga})$ ratio in the vapour phase.
For In$_{x}$Al$_{1-x}$P / ... / Ge a 0.005 Å fall at the dependence according to values calculated by Vegard law was detected. For A$_{x}$B$_{1-x}$C solid solution composition identification photoluminescence (PL) measuring was applied (spectra vs the heterostructure band gap according the solid solution composition). The obtained spectral maps (figure 4a) show the PL distribution of integrated intensity, the wavelength peak, the intensity peak and the width value at a half the spectrum height on the epitaxial structure (figure 4b).

Growth process, data maps visualization in comparison with the MOCVD reactor allows us to give a properties uniformity estimation and to reconstruct the growth parameters (figure 5).

The band gap value during PL spectra was estimated by:

$$E_g = \frac{hc}{\lambda}$$

(3)

where $E_g$ – photon energy, eV, $\lambda$ – photon wavelength (PL characterization), nm, $h$ – Planck constant, eV/s, $c$ – velocity of light, m/s.

**Figure 3.** Dependence of the In$_{x}$Al$_{1-x}$P epitaxial layers lattice parameter versus the In / (Al + In) ratio in the vapour phase: squares - InAlP / GaAs; circle - InAlP / InGaP / Ge; triangle - structure InAlP / GaAs / Ge; the dotted line - calculated according to Vegard law on GaAs; the straight line - calculated according by Vegard law on Ge; dash dotted line - Ge lattice parameter; dotted line - GaAs lattice parameter value.

**Figure 4.** Spectral map and single PL spectrum for one sample: a - the spectral map, b - the unit peak of the PL.
Figure 5. Steps of PL maps creation: a - combined maps visualization of several plates for a single growth in comparison with the MOCVD reactor construction, b - comparison of the several processes samples linear profiles (the square points - the profile for the case with two spaced peaks, triangular - for the case with one sharp peak and one wide peak, phomboid-shaped - for the case of two closely spaced peaks).

The epitaxial layer composition (for Ga$_x$In$_{1-x}$P at X <0.63) was calculated by:

$$E_g = 1.34 + 0.69 \cdot x + 0.48 \cdot x^2$$

The investigation data offered a picture of the uniform PL spectra peaks distribution over the sample surface. The PL spectra maxima range was not more than 2.8 %.

Such method is easier to use, the equipment offers possibility to get maps for the analysis of the properties uniformity. After both methods PL peaks distribution and XRD results comparing for In / (In + Ga) ratio in the solid phase with Si and Te doping (figure 6), it was detected a good correlation, so it proves the usage possibility.

Figure 6. In / (In + Ga) ratio dependence of the In$_x$Ga$_{1-x}$P epitaxial layer in the solid phase, from the XRD and PL on the ratio in the vapour phase methods: dots - the data from the XRD method; triangular points - the data from the PL method, the straight line – calculated based the table data according to the Vegard law.

4. Conclusion
We would like to point out main conclusions based on experimental: 1) In$_x$Ga$_{1-x}$P solid solutions with X- 45 - 53 % and In$_x$Al$_{1-x}$P with X- 46 - 51 % were grown as a single-crystal high quality multicomponent nanoheterostructure; 2) it was detected that the diffraction X-ray peaks showed a small broadening (less than 200 angular seconds); 3) it was found that the diffraction maxima mismatch and the diffraction peak broadening both can be used as parameters for the grown structure quality estimation.

Current data gives possibility for further step to the optimal technological parameters understanding for the perfect In$_x$Al$_{1-x}$P and In$_x$Ga$_{1-x}$P epitaxial layers growth for the cascade high-efficiency SC for space applications.
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