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Fields of deformation anisotropy exploration in multilayered (In,Ga)As/GaAs structures by high-resolution X-ray scattering

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The results of investigation of $In_{0.3}Ga_{0.7}As/GaAs$ superlattice by high-resolution X-ray scattering are presented. The influence of lattice distortion on diffraction curves (DC) were analyzed with dynamical diffraction theory. It allowed to explain azimuth dependence of experimental diffraction curves. Anisotropic changes in the shape of InGaAs lattice unit cell were shown and measured. The influence of smooth borders between hetero-layers were analyzed. Comparative analysis of different gradient functions on the hetero-border influence on diffraction curves was done. Parameters of heterojunction in investigated samples were determined with the help of DC modelling.

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1 Introduction

The task of grown superlattice structure definition is far from unequivocal realization and isotropic methods of the multilayered structures analysis widely applied today can yield doubtful results about sample structure. The influence of miscut on diffraction curves (DC) is well known [1] but it is usually accompanied by additional local layers misorientation [2]. Layers with different lattice parameters could minimize its strain energy by anisotropic deformation in unit cell [3]. If this fact is not considered, some false conclusions about investigated structure could be made. Besides, azimuthal scanning of the sample could give additional information from DC. This fact is described before [2, 3], but not for so small miscut angle and not all parameters were determined.

Extra information that could be obtained from DC analysis is structure gradient between layers with different composition [4]. The penetration depth and the shape of this gradient could be obtained from curves intensity analysis.

2 Experimental technique

All investigated samples were grown on thick GaAs substrate (100 oriented) with MBE and consisted from 17 periods of $In_{0.3}Ga_{0.7}As/GaAs$ layers with thicknesses 33/189 angstroms. More information about these samples could be found in [5].

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X-Ray diffraction curves were measured in the range of 3° in the vicinity of the exact Bragg position using so-called $\omega/2\theta$ mode for 400 reflection on double-crystal spectrometer (GaAs(100) crystal as monochromator, Cu Kα radiation). DC were measured for 0°, 45°, 90°, 135°, 180°, 225°, 270°, 315° azimuth angles with respect to [110] direction.

All information about the structure was obtained by experimental and simulated diffraction curves comparison.

3 Azimuthal dependend diffraction curves modeling

On the Fig. 1 two pairs of experimental and simulated DC for azimuthal angles 90° and 270° are shown. It is seen that the distance between satellite peaks are different for different azimuthal angles. This fact is due to structure miscut, in our case it makes up about 40 angular minutes. Zero satellite peak is also shifted, and to explain this fact an assumption about local misorientation in layers with larger lattice parameter of considered multilayered structure could be done.

In Fig. 2a) a model of lattice distortion is shown and in Fig. 2b) a distorted unit cell of InGaAs and undistorted unit cell of GaAs are shown. The lattice parameter of InGaAs is larger then for GaAs, so such deformations are efficient for minimization of strain energy (b_t on Fig. 2b) is larger then a). Moreover such deformations are not accompanied by dislocation generation.

To prove such anisotropic lattice distortion experimental diffraction curves for all azimuthal angles of scanning were compared with simulated. Good fitness of main maximums in DC was observed for the whole range of azimuthal angles.

Diffraction curves were simulated with plane-waves method [6] that is quite adequate for planar structure and with Takagi–Taupin approach [7] that gave the same result. Wave vectors in crystal were calculated numerically [8]. Azimuthal scanning was simulated by changing misorientation angle of InGaAs layers and miscut angle of the whole structure on sin law. These angles influence on the angles between local diffraction vectors $\boldsymbol{h}$ for each layer and surface normal. The results obtained were checked by native 3d modelling with the help of improved n-Beam modelling technique proposed by Stetsko & Chang [9] that will be described in [10]. This approach operates with x, y and z projections of wave vectors so it is very easy to obtain azimuthal DC. The results of this technique and two previous were completely the same.

From Fig. 1 it is seen that with such simulation technique good fitness of main satellite peaks angular position and intensity (more details are described in the next chapter) could be achieved. But experimental intensity between main peaks is much higher than for simulated curves. This is due to dispersion of layers thickness in each of 17 periods [11] and because of presence of defects in considered structure. These facts also explain the absence of small oscillations between main peaks. To take into account those effects diffuse scattering has to be considered, but for described in this paper anisotropy examination

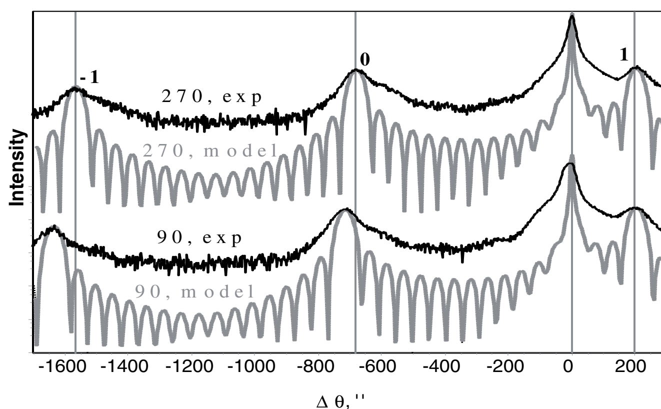

Fig. 1 Experimental (black) and simulated (grey, smooth) DC for azimuthal angles 270° (2 upper curves) and 90° (2 lower curves).

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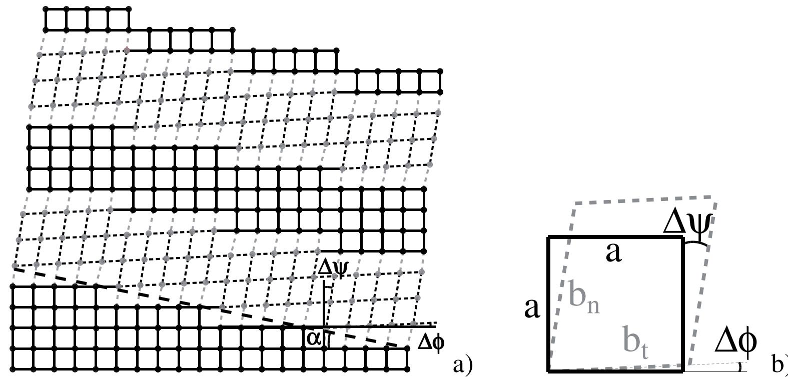

Fig. 2 Model of lattice distortion in the $In_{0.3}Ga_{0.7}As/GaAs$ sample with miscut. Black and solid – GaAs atoms, gray and dashed – InGaAs atoms. a) the whole layered structure, b) unit cells. Here α – is misut angle, a – is lattice parameter of GaAs, b_n and b_t – are normal and tangential lattice parameter of strained InGaAs, $\Delta\psi$ and $\Delta\phi$ – are normal and tangential misorientation angles for InGaAs lattice planes.

proposed dynamical calculation is quite enough, because anisotropic parameters of the sample were determined from angular position of main peaks.

From analysis of DC for 400 reflection the miscut angle is $\alpha = 40$ angular minutes and $\Delta\phi = 145$ angular seconds. To measure angle $\Delta\psi$ analysis of asymmetrical reflections must be done. Unfortunately 224 and 311 scans of these samples were rather bad quality, so it is hard to determine this angle with good accuracy, by it is about 1°.

4 Gradient on layers interface

From comparing simulated and experimental DC the information on interface between layers could be obtained. This would be demonstrated on diffraction curves for structure consisted from thick GaAs substrate (100 oriented) with MBE grown 8 periods of $In_{0.2}Ga_{0.8}As/GaAs$ layers with thicknesses 40/113 angstroms. Experimental diffraction curves were taken from work [12] where more information about these samples could be found. Described above technique was also applied for described below sample, but because of that sample imperfection the fitness between experimental and simulated curves could be achieved only for main satellite peaks.

To simulate smooth interface layers were broken into much thinner sublayers with different normal layer parameters and polarizability (more details could be found in [4]).

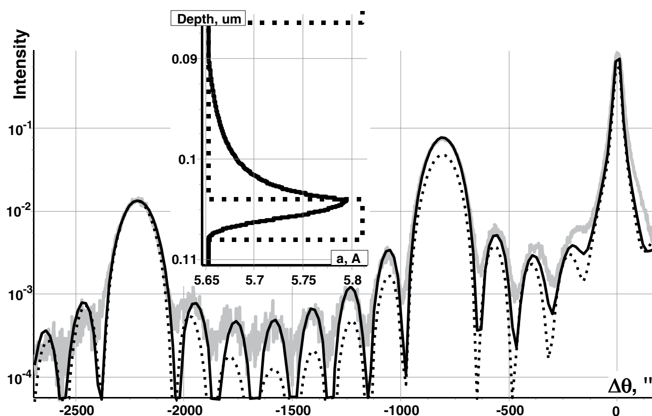

Fig. 3 Experimental DC (grey) for 311 reflection: model with sharp gradient (black, doted) and hyperbolic gradient (black, solid). On the insert lattice constant in angstroms on x-axis and the depth of sublayer in um as y-axis: solid – hyperbolic gradient, doted – sharp borders.

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By trying different laws of In concentration changing between InGaAs and GaAs layers the properties of interfaces were found (see insert on Fig. 3). As could be seen from Fig. 3 good intensity correlation between experimental and simulated DC could be achieved.

5 Conclusion

If smooth hetero-borders and anisotropic distortions in unit cell are not considered, wrong determination of structure parameters (both period of superlattice and ratio of layers thicknesses) may occur.

From azimuthal scanning of samples information about anisotropic deformations of lattice unit cell could be obtained. Such anisotropic deformations occur even for very small miscut angles (less then a degree). From examination of asymmetric scans all parameters of distorted unit cell could be found.

By analysing diffraction curves intensities information on hetero-border interface could be obtained.

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