P26

THE CRYSTALLOGRAPHIC STRUCTURE OF CATALYTICALLY GROWN ZnTe AND ZnMgTe NANOWIRES

E. Dynowska [1*], W. Szuszkiewicz [1], J.Z. Domagala [1], E. Janik [1], T. Wojtowicz [1], and W. Caliebe [2]

[1] *Institute of Physics, Polish Academy of Sciences, al. Lotników 32/46, 02-668 Warszawa, Poland*
[2] *Hasylab at DESY, Notkestr. 85, D-22603 Hamburg, Germany*

Keywords: nanowires, ZnTe, MBE technology, x-ray diffraction, synchrotron radiation

**) e-mail: dynow@ifpan.edu.pl*

One-dimensional semiconductor nanostructures in the form of free-standing nanowires (NWs) have become the focus of many research laboratories over the last years due to their use in basic physics investigations, as well as due to their potential applications in electronics and photonics devices. Using modern epitaxial growth techniques and the substrates activated by catalyst drops, NWs with radii of the order of tens of nanometers and lengths up to tens of micrometers can be obtained.

In this paper we describe the structural properties of ZnTe and ZnMgTe NWs grown by molecular beam epitaxy (MBE) using the (100), (110) and (111)-oriented GaAs substrates covered by gold/gal eutectic droplets serving as nanocatalysts. The NWs had diameters ranging from 30 to 70 nm and lengths between 1 and 2 μm [1,2]. The detailed characterization of the NWs by: field emission scanning electron microscopy (FE-SEM), high resolution transmission electron microscopy (HRTEM), energy-dispersive x-ray spectroscopy (EDXS) and x-ray diffraction (XRD) was previously reported. The FE-SEM and HRTEM studies shown that, independently on the orientation of the GaAs substrate, ZnTe NWs grow preferentially along <111>-type directions of the substrate and their growth axis is also <111>.

The main topic of this paper are the results of XRD studies. The measurements were performed using synchrotron radiation at the W1.1 beamline at DESY-Hasylab. The monochromatic x-ray beam of wavelength λ = 1.54056 Å was used. Two modes of measurement were applied: symmetrical ω-2θ scan and coplanar 2θ scan in the glancing incidence geometry. In the first mode of measurement the detector position (2θ angle) was coupled with the maximum intensity of the proper rocking curve (ω angle) resulting from the crystallographic orientation of the GaAs substrate. Such measurement allows to detect the lattice planes of NWs parallel to the crystallographic orientation of the substrate. In the second mode of measurement the rotational axis of the sample (ω axis) has been aligned exactly with the sample surface and then the sample was rotated about this axis by a very small angle α (here equal to 1º). During measurement the angular position of the sample with respect to the incident x-ray beam (α) was fixed while the detector was rotated in the wide range of 2θ angles in the plane perpendicular to the sample surface. Such technique is very sensitive to very thin layers. The examples of the diffraction patterns obtained in this two modes for ZnTe NWs grown on GaAs (001)-oriented substrate are shown in Figs. 1 and 2.

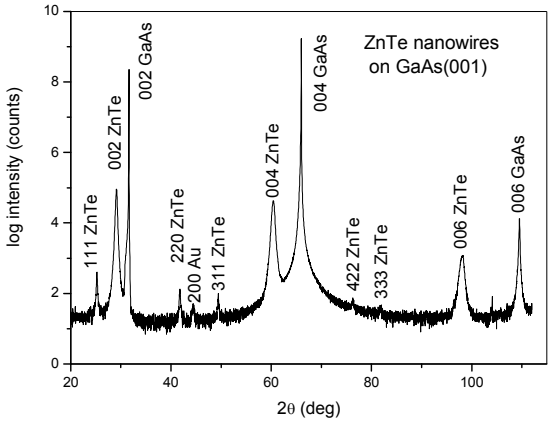

Figure 1. The x-ray ω-2θ scan obtained for ZnTe NWs grown on (001)-oriented GaAs substrate.

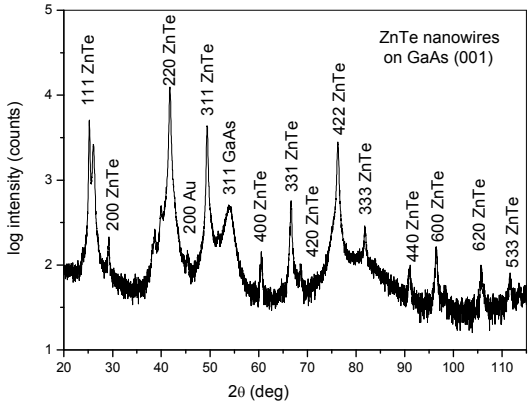

Figure 2. The x-ray 2θ scan obtained in glancing incidence geometry for ZnTe NWs grown on (001)-oriented GaAs substrate.

P26

Analysis of the ω-2θ pattern shows that the crystallographic orientation of the substrate imposes the orientation of the NWs: the strongest among observed reflections of ZnTe are indexed 002, 004 and 006, respectively, which correspond to analogous reflections of the GaAs substrate. This means that the (100) lattice planes of the NWs are parallel to the (100) lattice planes of the substrate. Additional small peaks visible in Fig. 1 (*e.g.* indexed as 111, 220, 311…), as confirmed by 2θ scan performed in the glancing incidence geometry (Fig. 2), originate mainly in the thin polycrystalline layer of ZnTe that forms directly on the GaAs substrate between the NWs.

The measurements performed for the NWs grown on (110) and (111)-oriented GaAs substrates lead to similar conclusions confirming the epitaxial relation between the substrate and the growing NWs.

The important question is the crystal structure of NWs. Detailed structural information concerning the single ZnTe NWs was obtained from HRTEM studies. Electron diffraction from a large number of the NWs reveals pattern characteristic for the zincblende (ZB) crystal structure with lattice parameter a = 0.61 nm [2]. This value, within frames of accuracy typical for electron diffraction, seems to be the same as that for bulk ZnTe (a = 0.6103 nm). However, on the base of x-ray diffraction measurements, the ZB lattice parameter of ZnTe NWs calculated from symmetrical reflections 400, 440 and 333, respectively, was slightly larger than that for bulk ZnTe and equals to a = 0.6112 nm for (100)-oriented substrate, a = 0.6107 nm for (110)-oriented substrate and a = 0.6109 nm for (111)-oriented substrate (all values are obtained with accuracy of ± 0.0002 nm).

In order to explain such results we assumed that the real unit cell of NWs has to be deformed along the [111] crystallographic direction of zincblenede unit cell. Such deformation would lead to the rhombohedral unit cell. We suppose that the source of such deformation is the special defect structure inside NWs visible in the HRTEM studies. According to these results for the majority of NWs the bottom part reveals a high number of stacking faults and/or microtwins [2]. As a result the mean interplanar spacing along [111] direction changes leading to rhombohedral distortion of the ZB unit cell. To check this supposition we have undertaken an attempt of lattice parameters calculation of such distorted unit cell.

As it is known, the rhombohedral unit cell is characterized by two lattice parameters a and α, where $a = b = c$, $\alpha = \beta = \gamma \neq 60°$. So, the knowledge of at least two different interplanar spacing is necessary for description of such crystal structure. In our calculations we used the interplanar spacing calculated from x-ray ω–2θ scans obtained for differently oriented ZnTe NWs, d_{400}, d_{440} and d_{333}, changing properly their *hkl* indexes. We assumed that the defect structure has the same character in all these NWs, so the unit cell distortion should also be the same. The *hkl* indexes transform to the defined above rhombohedral unit cell as follows: from 400 in cubic cell to 220, from 440 – to 422 and from 333 – to 333, respectively. Next, we have calculated rhombohedral lattice parameters of ZnTe NWs, solving the system of equations proper for rhombohedral crystals for d_{220} and d_{422} values. We obtained the lattice parameters a = 0.4320 ± 0.0004 nm and α = 60.06 ± 0.01°. In order to check the correctness of this result we calculated the d_{333} value for this unit cell and compared this with the experimental d_{333} value obtained for (111)-oriented ZnTe NWs – these values are the same within the accuracy of 0.0001 nm. Therefore, we believe that the procedure used for above calculations is correct. Similar calculations performed for ZnMgTe NWs grown on the (100) and (110)-oriented GaAs substrates gave the rhombohedral unit cell with parameters: a = 0.4353 ± 0.0004 nm and α = 60.04 ± 0.01°. On the basis of the above result we can state that the shape of the unit cell is the same as in the case of ZnTe NWs (the angle α is practically the same in both cases), while the a parameter is larger due to bigger size of Mg atoms built in ZnTe lattice.

Summarizing, we can say that in the light of x-ray studies the crystal structure of ZnTe NWs differs from that in the bulk material: due to the defect structure created during growth of NWs the ZB unit cell is distorted to the rhombohedral one.

Acknowledgements:

This research was partially supported by the Ministry of Science and Higher Education (Poland) through Grants N507 030 31/0735 and N515 015 32/0997, and by the Network "New materials and sensors for optoelectronics, information technology, energetic applications and medicine", as well as by the European Community - Research Infrastructure Action under the FP6 "Structuring the European Research Area" Programme (through the Integrated Infrastructure Initiative "Integrating Activity on Synchrotron and Free Electron Laser Science", Contract RII3-CT-2004-506008).

References

[1] E. Janik, J. Sadowski, P. Dluzewski, S. Kret, L.T. Baczewski, A. Petroutchik, E. Lusakowska, J. Wróbel, W. Zaleszczyk, G. Karczewski, T. Wojtowicz, A Presz, "ZnTe nanowires grown on GaAs (100) substrates by molecular beam epitaxy", *Appl. Phys. Lett.* **89** (2006) 133114.

[2] E. Janik, P. Dłuzewski, S. Kret, A. Presz, H Kirmse, W. Neumann, W. Zaleszczyk, L.T. Baczewski, A. Petroutchik, E. Dynowska, J. Sadowski, W. Caliebe, G. Karczewski, T. Wojtowicz, "Catalytic growth of ZnTe nanowires by molecular beam epitaxy: structural studies", *Nanotechnology* **18** (2007) 475606.