Thermal expansion of GaN in the temperature range 10 K - 296 K

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Nitrides of group III metals (wurtzite-type AlN, GaN, InN) are, at present, one of the most intensively studied families of semiconductors, due to their potential applications in short-wave optoelectronics (from green to ultraviolet). One of the recent achievements is the continuous-wave operation of (In,Ga)N multiquantum-well structure laser diodes with a lifetime of 27 hours [1].

Most applications of group-III nitrides involve the thin-layer technology. Due to lattice mismatch and to differences in thermal expansion coefficient (TEC) values of the layer and of the substrate, the layers are strained. As the physical properties of the layer are strain-dependent, the knowledge of the thermal expansion is required. In particular, the knowledge of lattice constants at high temperatures and thermal expansion coefficient is of high importance, because they are used in calculation of strain in binary layers and in determination of composition of solid solutions such as (In,Ga)N.

The generally accepted room temperature lattice-parameter values of GaN are $a = 3.182(9)$ Å, $c = 5.1850(5)$ Å [2]. However, detailed investigations of gallium nitride single crystals show that their values at the gallium side are by about 0.001 Å larger than at the nitrogen side [3]. Discrepancies are encountered between the TEC values of GaN and there is a lack of detailed studies at low temperatures: only some experimental points have been reported for the helium (from 40 K) and nitrogen cryotemperatures. The literature data on TEC at the room temperature exhibit a considerable scatter from $2.8 \times 10^{-6}$ K$^{-1}$ [4] to $5.59 \times 10^{-6}$ K$^{-1}$ [5] in $a$ direction, and from $3.1 \times 10^{-6}$ K$^{-1}$ [4] to $3.7 \times 10^{-6}$ K$^{-1}$ [6] in $c$ direction.

The measurements were carried out at a high-resolution X-ray powder diffractometer (B2 beamline at HASYLAB) equipped with helium cryostat. Debye-Scherrer geometry with rotating capillary was applied. In this work the GaN fine powder synthesised at Warsaw University of Technology by reaction of metallic indium with ammonia was studied. The sample was mounted within a thin wall capillary of 0.5 mm diameter. 15 intense peaks in the range $25° < 2θ < 140°$ were measured (using $λ = 1.20070$ Å and stepwidth 0.01°) and applied in the least-squares refinement. The reflection profiles were fitted assuming the gaussian shape.

The aim of the present study was the determination of the lattice constants values for GaN powder in the temperature range from 10 K up to 296 K. The measurements performed show (see Fig. 1) that the thermal expansion in both $a$ and $c$ directions is close to zero below about 100 K. The $a(T)$ run shows a shallow minimum at about 100 K. For comparison, the temperature dependence reported for the gallium side of a GaN single crystal in [3] and the room temperature values reported in [2,7] are shown in Fig. 1 in the range 40 K - 400 K. The observed discrepancies in lattice parameter values in relation to results obtained for single crystals are attributed to effects of strain and defects (see the discussion in [7]).

References

Figure 1: Lattice-parameter dependence on temperature (empty squares - powder data, this work; filled squares - single crystal data [3]). The solid lines represent the best fit to the experimental data using quadratic polynomial. Triangles refer to the room temperature values [2], crosses illustrate the difference between the two sides of a single crystal at room temperature [7].


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