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Influence of the columnar structure of heteroepitaxial nitride layers on the transport of electrons

A. SZYSZKA*, B. PASZKIEWICZ, R. PASZKIEWICZ, M. TŁACZAŁA

Faculty of Microsystem Electronics and Photonics, Wrocław University of Technology,
ul. Janiszewskiego 11/17, 50-372 Wrocław, Poland

The influence of the columnar structure of heteroepitaxial nitride layers on electronic transport has been described within the model of thermionic emission of carriers through potential barriers formed at grain boundaries. Dependence of the potential barrier height on the material properties and applied external voltage has been calculated. Potential barriers heights for gallium nitride layers grown by the metalorganic vapour phase epitaxy method has been estimated to be in the range of 20–60 meV and 10–40 meV in the dark and under illumination, respectively.

Key words: *gallium nitride; columnar structure; electronic transport*

1. Introduction

Gallium nitride and its alloys are applied for fabrication of UV light detectors and emitters and for high frequency, high power field effect transistors. Despite a great progress in device technology, the highest predicted and calculated parameters of fabricated structures have not been obtained. Discrepancies between the theoretical and obtained parameters of the devices are mainly caused by an assumption that heteroepitaxial layers of A(III)N compounds have singlecrystalline structure. This assumption neglects the fact that epitaxial layers of nitrides always have columnar structure with low angle boundaries. Distribution of sizes of crystallites in heteroepitaxial layers grown by metal-organic chemical vapour deposition (MOCVD) method was examined by high resolution X-ray diffractometry [1]. It was shown that sizes of crystallites in a layer depend on conditions of the growth process and that GaN layers grown on sapphire substrates consist of crystallites of various sizes.

Dangling bonds and atoms of impurities existing in disordered boundary area introduce deep trap levels in the forbidden band of the material. Negatively charged

*E-mail: adam.szyszka@pwr.wroc.pl

acceptor traps, in n-type material, form potential barriers for a majority of carriers. Influence of these barriers on the surface potential in GaN layers was examined by the scanning Kelvin probe microscopy [2]. Nonuniformity of photocurrent flow in AlGaN MSM detectors, caused by columnar structure of the layer, was observed by the light beam induced current technique [3].

2. Calculations

One-dimensional model which allowed the analysis of the formation of potential barrier at the grain boundary was evaluated (cf. [4–7]) in order to describe electronic properties of polycrystalline silicon.

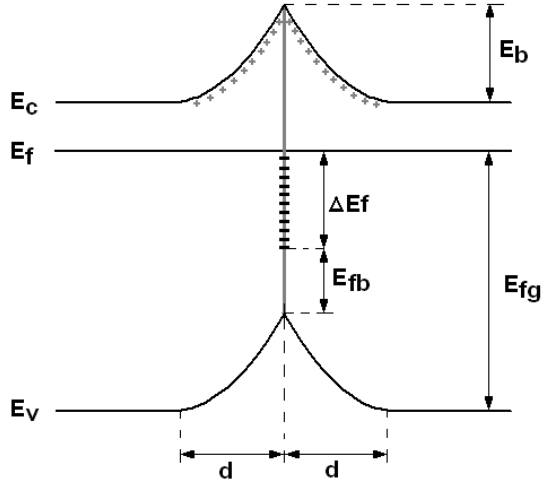

Fig. 1. Scheme of the energy band diagram of a potential barrier formed at the boundary of two grains: E_f – Fermi energy level, E_b – potential barrier height, E_{fg} – Fermi energy level in the volume of a grain, E_{fb} – Fermi energy level in grain boundary in neutral conditions, ΔE_f – shift of the Fermi level at the grain boundary caused by the excess charge ($\Delta E_f = E_{fg} - E_{fb}$), d – width of the space charge region

The energy band diagram of two adjacent grains in a semiconductor is presented in Fig. 1. The model assumes a constant distribution of densities of deep trap states at the grain interface. The negative charge associated with interface trap states is balanced by the positive net charge of uncompensated ionized shallow donor states. Donor states occur in GaN layers mainly due to the presence of N vacancies. Non-compensated donor states are localized in space charge regions created on both sides of the grain boundary. The height of the potential barrier depends on the relation between density of the interface states and concentration of donor states in the grains. It could be concluded (Fig. 2) that for higher values of the concentration of shallow donors in the volume of a grain (N_d), a higher density of acceptor trap states at the grain boundary (N_T) is needed to form the potential barrier. We have also found that for very

high values of trap densities at the grain boundary, the potential of the barrier was pinned and was dependent only on E_{fb}.

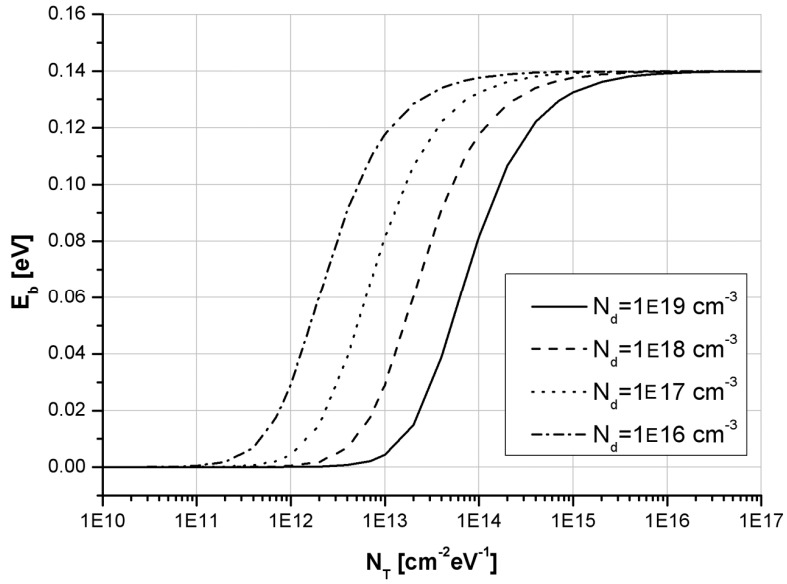

Fig. 2. Dependence of the calculated height of the potential barrier on the trap states density at grains boundary for various concentrations of donors in the grains (the calculation was carried out for E_{fb} = 3.1 eV)

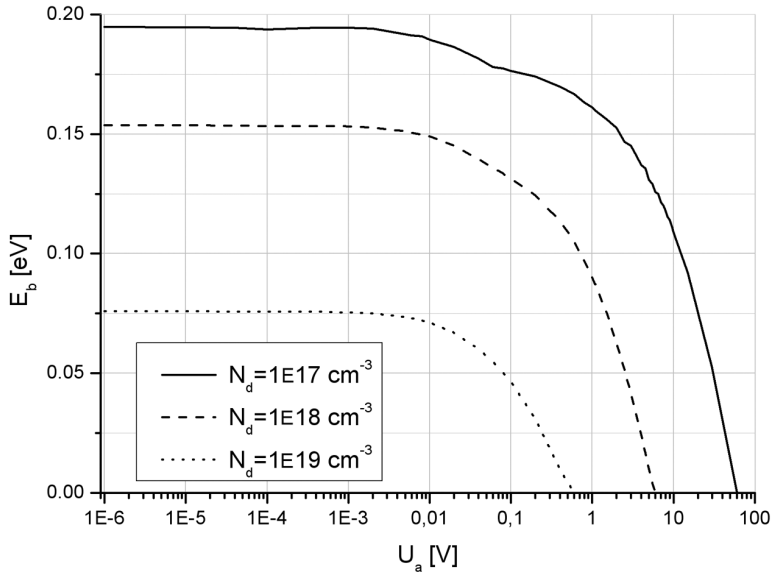

Fig. 3. Dependence of the calculated height of the potential barrier on the applied voltage at grains boundary for various concentrations of donors in the grains (the calculation was carried out for E_{fb} = 3.02 eV)

The calculated dependence of the height of the potential barrier on the external voltage is presented in Fig. 3. The N_T value at the grain boundary was assumed to be 4×10^{17} $cm^{-2}\cdot eV^{-1}$ based on Refs. [8] and [9]. For small values of the applied voltage the barrier height remained constant. Further, with subsequent increase of the voltage, the barrier height started to decrease to the point where it vanished for a defined value of voltage. The breakdown voltage of the potential barrier was higher for the higher initial barrier height. After reaching the breakdown voltage, the conductivity of the layer was controlled only by bulk conductivity of grains. This effect could explain the observed phenomenon that despite small mobility of electrons in heteroepitaxial layers of nitrides, the measured drift velocity of electrons in high electric fields is very high [10].

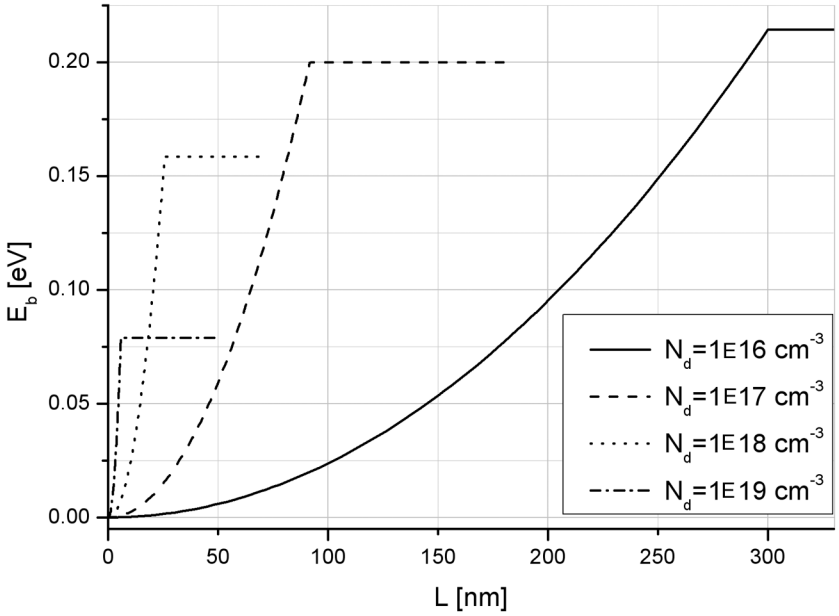

Fig. 4. Influence of the size of grains on the potential barrier height for various concentrations of donors in the grains

The dependence of the potential barrier height on the sizes of grains is presented in Fig. 4. It was observed that decrease of grain sizes did not influence the potential barrier height till the point when it reached the value equal to the double width of the space charge region. This occurs when the space charge regions occupy the whole grain. Further decreasing of the grain sizes caused the decrease of the barrier height due to overlapping of the depletion regions. These phenomena could be responsible for spatial non-uniformities in photo-response of AlGaN MSM detectors [3].

The dependence of the barrier height on the concentration of donors in grains is presented in Fig. 5. In the area of small donor concentration, its increase caused the increase of the barrier height due to an increase of the number of electrons trapped at the grain boundary. When all interface states were completely filled, the potential

barrier height reaches its maximum. Further, any increase of the concentration of donors results in a decrease of the barrier height due the increase of the compensating positive charge of ionized donors in the depletion layer.

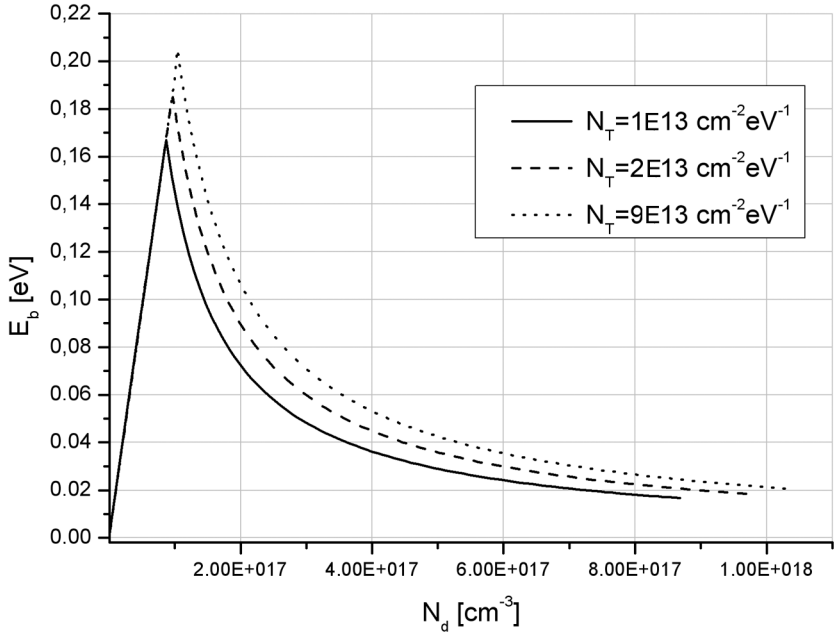

Fig. 5. Dependence of the calculated potential barrier height on the concentration of donors in the grains (calculation was carried out for E_{fb} = 3.02 eV)

3. Experiments

The potential barrier heights in MOVPE gallium nitride layer have been estimated based on the measurements of the temperature dependence of conductivity of the epitaxial layer (Fig. 6). Assuming a thermionic character of emission through potential barriers, their heights could be evaluated from the slope of the Arrhenius plot of the conductivity vs. temperature. Two values of barrier heights of the GaN heteroepitaxial layer were measured: one for dark conditions, the other for an illuminated sample. Potential barrier heights have been estimated to be in the range of 20–60 meV for the former case and 10–40 meV for the latter one. The decrease of the potential barrier heights for an illuminated sample could be explained by a release of electrons from the trap states caused by the incident photons. That also could explain another specific behaviour of nitride layers, namely the persistent photoconductivity. Presumably, photo-generated electrons could not re-occupy deep states because of the existence of residual negative charge at grain boundaries repelling electrons. Thus grain boundaries remain lowered for a long time after switching off the illumination.

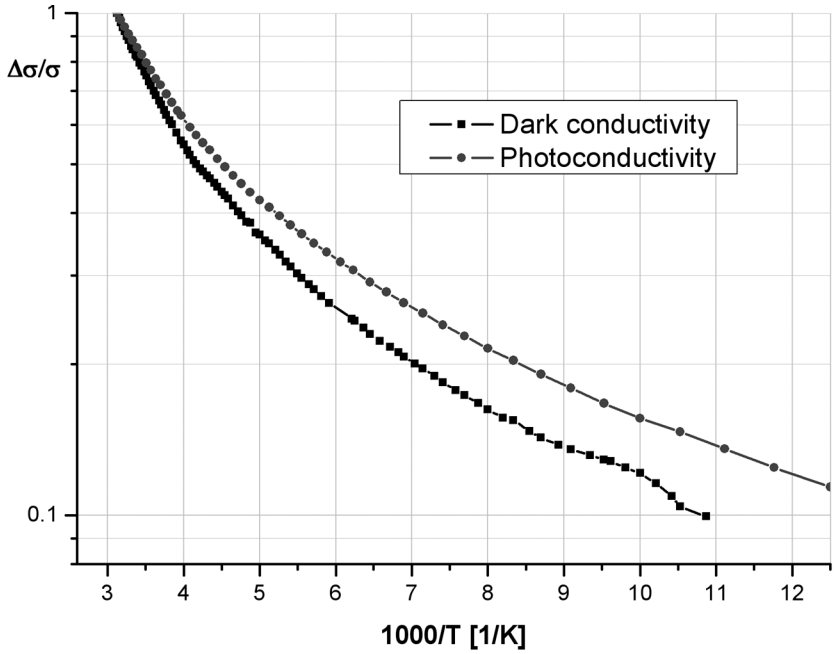

Fig. 6. Temperature dependence of conductivity of GaN heteroepitaxial layer

The nonlinearity of the Arrhenius plot observed in the low temperature region could indicate the occurrence of other conduction phenomena in nitride layers such as tunneling effect and/or impurity band conduction.

4. Conclusions

The model of formation of potential barriers at the grain boundaries of heteroepitaxial layers of nitrides has been put forward. The dependence of the barrier height on the layer parameters such as the density of deep traps, concentration of shallow donors, energy of Fermi level at grain boundary in neutral conditions and the size of grains has been calculated. The presence of potential barriers at grain boundaries allowed us to explain some characteristic properties of nitride heteroepitaxial layers. Potential barrier heights of MOVPE GaN layers were calculated based on the dependence of conductivity vs. temperature with an assumption of the thermionic character of the emission.

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