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Structural and Optical Properties of Wurtzite AlGaAs Nanowires Grown by MBE on Si(111) Substrate¹

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Abstract—We present the results of photoluminescence measurements of Al_xGa_{1-x}As nanowires, together with the transmission electron microscopy structural analysis. Al_xGa_{1-x}As nanowires were grown by molecular beam epitaxy under the nominal aluminum contents $x = 0.3–0.7$. The obtained results demonstrate the presence of wurtzite structure in Al_xGa_{1-x}As nanowires.

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While the bulk GaAs and Al_xGa_{1-x}As crystals have a zinc blende (ZB) structure, both ZB and wurtzite (WZ) structures can be observed in GaAs and Al_xGa_{1-x}As nanowires (NWs). Experimental and theoretical results show that the band gap energies are different for WZ and ZB A₃B₅ NWs, that is their optical properties are expected to differ significantly. Thus, WZ NWs can be considered as a new semiconductor material, and the study of its optical properties has a fundamental interest for semiconductor physics. The transmission electron microscopy (TEM) data confirm the presence of a WZ phase in Al_xGa_{1-x}As NWs, but the results of experimental studies of their optical properties, to the best of our knowledge, is not represented in the up-to-date literature. The optical properties of the structures based on Al_xGa_{1-x}As, depending on the value of x , have been studied in details as concerns to the bulk systems, while the similar studies for Al_xGa_{1-x}As NWs have not been carried out. There are only a few papers which deal with the optical properties of Al_xGa_{1-x}As NWs [1–3]. It is worth to notice, that a possible presence of a WZ phase in the Al_xGa_{1-x}As NWs is not discussed in these papers. The influence of core-shell structure formed during the Al_xGa_{1-x}As NWs growth on their optical properties is not discussed up to now. Nevertheless, it is known that in the process of Al_xGa_{1-x}As NWs growth by molecular beam epitaxy (MBE), the spontaneously formed NWs have a relatively low Al content in the core but a higher Al content along the lateral faces (shell) [4]. The dimensions of the core and shell are such that the

quantum-size effects are not observed. In this work, the study of the optical properties of the Al_xGa_{1-x}As NWs array is presented. The photoluminescence (PL) measurements are compared with the structural properties of Al_xGa_{1-x}As NWs obtained by means of TEM and scanning electron microscopy (SEM). Nominal content of Al in the solid solution was varied within the range of $x = 0.3–0.6$ [4]. The Al_xGa_{1-x}As NWs array was synthesized using the MBE on a Si(111) substrate. The synthesis of the structure under investigation was described in detail in our works published earlier [1, 2, 4]. SEM measurements show that the pencil-like Al_xGa_{1-x}As NWs are formed during the MBE growth (Fig. 1). The results of TEM measurements reveal a WZ type structure for all Al_xGa_{1-x}As NW with nominal Al content in the range of $x = 0.3–0.7$ (Fig. 2). As it was concluded in our previous paper [5] the Al_xGa_{1-x}As NWs synthesized by MBE method form a core-shell structure with a sharp interface between core and shell. The results obtained by means of high-angular dark-field imaging and energy dispersive X-ray spectroscopy evaluate the Al content in the NW shell as about 0.55, which is nearly equal to the nominal Al content $x = 0.6$, contrary to Al content in the core about $x = 0.35$ [5]. The numerical calculations of Al content in the core and shell of Al_xGa_{1-x}As NWs are presented in [5] for the different nominal Al content. It is known, that ZB Al_xGa_{1-x}As is a direct band gap semiconductor for $x < 0.4$ but becomes the indirect band gap semiconductor for $x \geq 0.4$ [6]. The similar transformation is not known at the moment in the case of WZ Al_xGa_{1-x}As.

Thus, we investigate the optical properties of a new semiconductor structure, namely NWs with the WZ

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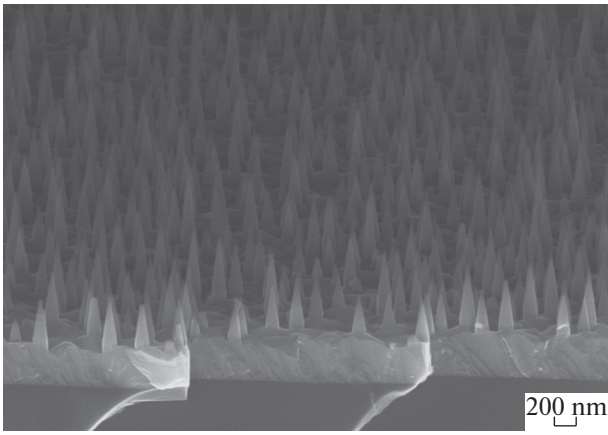


Fig. 1. SEM image of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ NWs with nominal content of Al $x = 0.7$.

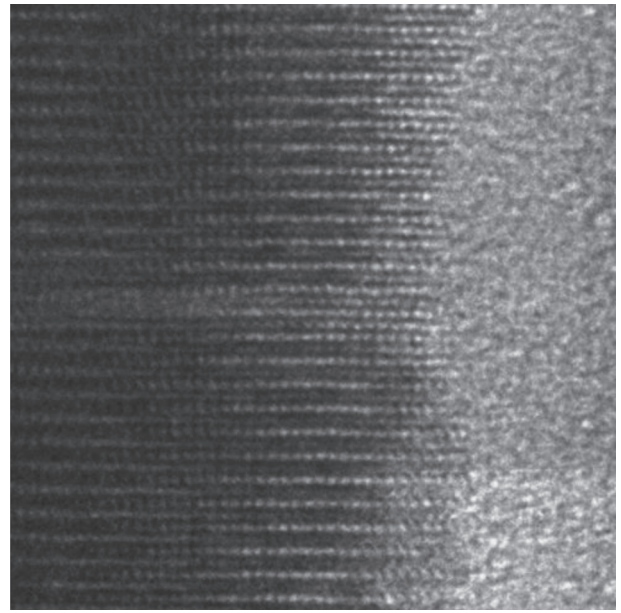


Fig. 2. TEM image $\text{Al}_x\text{Ga}_{1-x}\text{As}$ NWs with nominal content of Al $x = 0.4$.

phase predominance with the different values of x . We have considered the PL of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ NWs with a nominal content of Al in the range of $x = 0.3$ – 0.6 in our previous papers [1, 2]. The PL spectra excited by the photons with the energy 2.33 eV at 10 K. occur to differ significantly from the spectra of the bulk $\text{Al}_x\text{Ga}_{1-x}\text{As}$ with the same Al content [6]. In the present work we investigate the PL of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ NWs with the nominal value of $x = 0.7$.

We have to take in consideration not only the effects related to the change in Al content on the core-shell heterointerface but also the band gap difference

between WZ and ZB $\text{Al}_x\text{Ga}_{1-x}\text{As}$. These contributions explain the complex form of PL spectra for all our samples. The numerical simulation predicts that Al content in the core exceeds 0.4 in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ NWs with a nominal value of $x = 0.7$ [5]. Note, that in this case the bulk ZB $\text{Al}_x\text{Ga}_{1-x}\text{As}$ has the indirect band

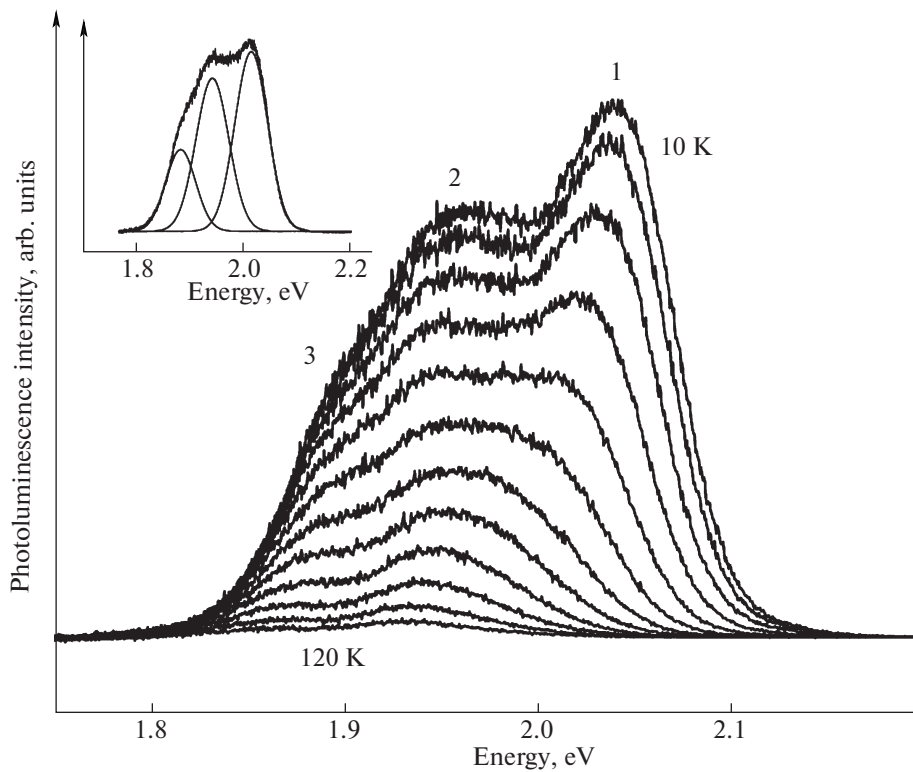


Fig. 3. Photoluminescence spectra of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ NWs at the temperature range 10–120 K.

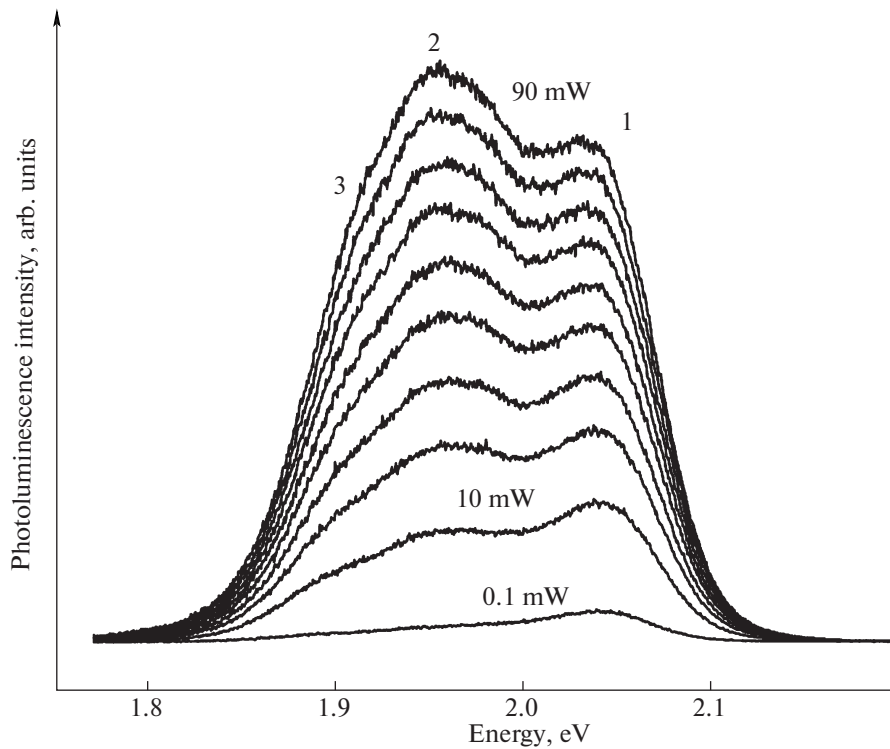


Fig. 4. Photoluminescence spectra of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ NWs with nominal content of Al $x = 0.7$ obtained at 0.1, 10–90 mW excitation powers. Laser spot diameter is 0.3 mm, $T = 5$ K.

gap [6]. We observe a significant transformation in the PL spectra for the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ NWs at the nominal value of $x = 0.7$, depending on the excitation level and temperature (Figs. 4, 5). Thus, it is possible that WZ $\text{Al}_x\text{Ga}_{1-x}\text{As}$ becomes the indirect gap semiconductor for Al content which exceeds 0.4, contrary to the theoretical predictions [7].

The PL spectra of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ NWs with the nominal value of $x = 0.7$ are depicted in Fig. 4. In our opinion, the high energy component 1 of these spectra can be attributed to the NW core-shell interface. Under the increasing temperature this component shifts towards the low energies, weakens and disappears about 70 K. Other components 2 and 3 are related probably, to the light emission from the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ NW core and the top part of the NW. Note, that it was shown in [5] that Al content decreases sharply near the top of NW. These peculiar properties of NWs may be the reason for the presence of two components 2 and 3 which contribution becomes relatively strong at high temperatures. This suggestion is supported by their intensity dependence on the excitation level (Fig. 4). The component 1 dominates under the low excitation, while the intensities of components 2 and 3 relatively increase under the high excitation. These changes can be explained by the saturation of the luminescence from the core-shell interface.

Further optical investigations of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ NWs will allow to determine the band gap difference between WZ and ZB $\text{Al}_x\text{Ga}_{1-x}\text{As}$, depending on the

value of x as well as the electron band structure of WZ $\text{Al}_x\text{Ga}_{1-x}\text{As}$.

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