

Theoretical analysis of compositional profiles in axial heterostructures based on AlGaAs nanowires

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We analyze the compositional profiles across axial heterostructures in GaAs/Al_xGa_{1-x}As/GaAs and Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As nanowires (NWs). The difference is in the catalyst type (Ga or Au) and in the material from which the heterostructure starts (binary GaAs NW or ternary Al_xGa_{1-x}As NW). We calculate the interfacial profiles and show that the use of Au catalyst significantly broadens the interface due to reservoir effect. This feature is experimentally confirmed.

Keywords: semiconductor nanowires AlGaAs, axial heterostructures, compositional profiles, modeling.

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Nanowire (NW) of triple semi-conducting compounds III–V (III–V NW) and heterostructures based on them are broadly used in basic research and various optoelectronics devices that can be combined with the silicon electronic platform [1–3]. Axial heterostructures $A_{x_0}B_{1-x_0}C/A_{x_s}B_{1-x_s}C/A_{x_0}B_{1-x_0}C$ in III–V NW $A_xB_{1-x}C$ with an initial composition of x_0 and a stationary composition of x_s are usually grown using the vapor–liquid–solid (VLS) mechanism. The reservoir effect associated with the residual concentrations of atoms of various elements in the drop leads to blurring of the axial heterointerfaces [4–7]. The classical Al_xGa_{1-x}As material system is one of the most important heteroepitaxial systems on the basis of which GaAs/AlGaAs axial structures of various compositions and crystal phases are synthesized in NW [8–14]. The purpose of this work is to theoretically study the composition profiles in double axial heterostructures based on AlGaAs NW and analyze the factors influencing the width of heterointerfaces in this system.

It is known from Ref. [6,15,16] that in order to calculate the composition profiles during the growth of the heterostructure by the VLS mechanism, the dependence of the composition of NW Al_xGa_{1-x}As x on the relative concentration of Al atoms in the drop of $y = \chi_{Al}/(\chi_{Al} + \chi_{Ga})$ catalyst is required. Hereafter, χ_k denotes the relative atomic concentrations of the elements $k = \text{Al, Ga, As, and Au}$ dissolved in a liquid that satisfy the condition $\chi_{Al} + \chi_{Ga} + \chi_{As} + \chi_{Au} = 1$. During selfcatalyzed growth of NW, we have $\chi_{Au} = 0$, while $\chi_{As} \cong 0$ in all cases, due to the low solubility of As in liquid at typical growth temperatures $\sim 500\text{--}630^\circ\text{C}$ [4,12,16,17]. According to the results of study in Ref. [18], the liquid–crystal distribution $x(y)$ during the VLS growth has an equilibrium character for ternary compounds III–V, based on the mixing of atoms of group III [15,16], and it has a kinetic character when atoms of

group V are mixed [17]. The equilibrium distribution $x(y)$ for the lattice-matched system Al_xGa_{1-x}As is determined by the Langmuir–McLean formula [18]:

$$x = \frac{c_l y}{1 + (c_l - 1)y}. \quad (1)$$

The c_l coefficient, which describes the differences in the affinity coefficients of Al and Ga atoms, depends on the value of $\chi_{tot} = \chi_{Al} + \chi_{Ga} \cong 1 - \chi_{Au}$ and the temperature [18] and decreases sharply with an increase in the concentration of Au in the drop (Fig. 1). The values of $c_l \gg 1$ correspond to the well-known property of the VLS growth of AlGaAs NW, according to which the concentration of Al atoms in a drop is much lower than the concentration of Ga atoms [15,16,18,19] (Fig. 1).

Assuming a constant rate of axial growth of NWs when switching flows of group III atoms, the Al composition in the drop y obeys the kinetic equation [19]:

$$\frac{1}{g} \frac{dy}{d\xi} = x_s - x. \quad (2)$$

Here, x_s — is the stationary value of the AlAs composition in the heterostructural insert, ξ — is the dimensionless coordinate along the axis of NW growth expressed in monolayers (ML), g — is the geometric parameter defined below. Using (1) in (2) and integrating with the initial condition $x(\xi - \xi_0) = x_0$, we obtain an analytical solution for the composition profile along the NW axis in the form

$$\begin{aligned} \frac{\xi - \xi_0}{\Delta\xi} = & \frac{1}{(1 - bx_s)^2} \ln \left[\frac{(x_s - x_0)(1 - bx)}{(x_s - x)(1 - bx_0)} \right] \\ & + \frac{b(x_0 - x)}{(1 - bx_s)(1 - bx_0)(1 - bx)}. \end{aligned} \quad (3)$$

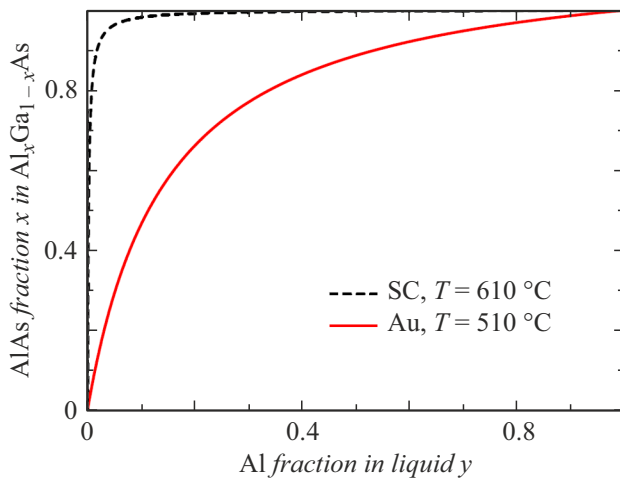


Figure 1. Al distribution in Liquid–crystal during growth of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ NW by the VLS mechanism during selfcatalyzed growth in the absence of Au at temperature of $T = 610^\circ\text{C}$ and Au-catalytic growth at $T = 510^\circ\text{C}$ and $\chi_{\text{Au}} = 0.5$. Calculation using the formula (1) for $c_l = 497$ and 7.8 , respectively [19].

The characteristic width of the interface $\Delta\xi$ for an NW with a radius R is

$$\Delta\xi = \frac{1}{g c_l} = F \frac{1 - \chi_{\text{Au}}}{c_l}, \quad F = \frac{\Omega_s R f(\beta)}{3 \Omega_L h}, \quad (4)$$

where

$$f(\beta) = \frac{(1 - \cos\beta)(2 + \cos\beta)}{(1 + \cos\beta) \sin\beta} \quad (5)$$

is a geometric function of the contact angle of the drop β at the top of the NW [7]. The values Ω_s , Ω_L and h denote the elementary volume per pair III–V in a solid, the elementary volume in a liquid, and the height of the monolayer, respectively. These values are well known for the AlGaAs system [16]: $\Omega_s = 0.0452 \text{ nm}^3$, $\Omega_L = 0.02 \text{ nm}^3$ and $h = 0.326 \text{ nm}$. We would like to note that the obtained solution describes the composition profile in any $A_{x_0}B_{1-x_0}C/A_{x_s}B_{1-x_s}C/A_{x_0}B_{1-x_0}C$ binary heterostructure in III–V NW with any initial composition x_0 and stationary composition x_s , provided that the liquid–crystal distribution is determined by formula (1).

Fig. 2 shows the AlAs composition profiles in the double axial heterostructures $\text{GaAs}/\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}/\text{GaAs}$ and $\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}/\text{GaAs}/\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}$ with geometric parameters from the table corresponding to the experimental data from Ref. [12] and Ref. [10] respectively, with the same 50% composition of AlGaAs sections. The remaining parameters in the table are calculated using formulas (4) and (5). Analysis of the calculated composition profiles shows that, with the same composition, the width of the interfaces weakly depends on the material from which the heterostructure begins to grow (binary GaAs in the first case and NW of triple composition $\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}$ in the second case). The temperatures difference is also not important. The main factor determining the increase in interface width

with these parameters is the presence of Au in the drop. This leads to a significant decrease in the c_l value from 497 for selfcatalyzed NW to 7.8 for Au-catalytic NW and, as a result, to an increase in the characteristic interface width from 3 to 15 ML (see the table). An increase in $\Delta\xi$ for Au-catalytic NW is observed even though the volume of droplets at their tip is significantly smaller due to the smaller radius and contact angle of the droplet.

Fig. 3 shows a comparison of calculated curves and experimental data on composition profiles for selfcatalyzed $\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ NW with $T = 610^\circ\text{C}$ [12] and Au-catalytic $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ NW with the initial composition $x_0 = 0.3$. The calculated parameters correspond to those shown in the table. It can be seen that

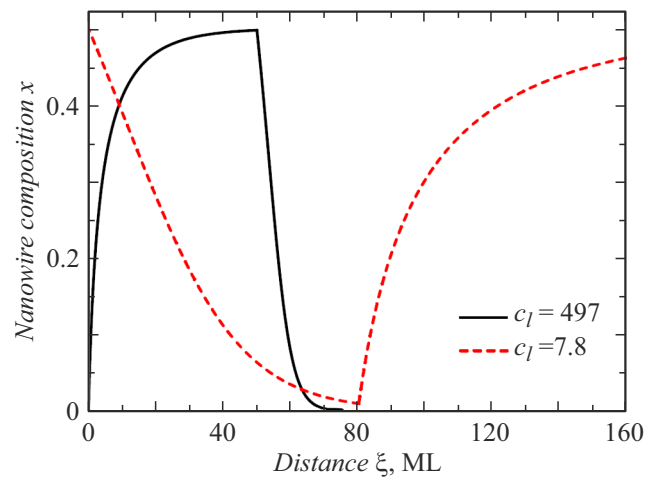


Figure 2. Composition profiles in double axial heterostructures in $\text{GaAs}/\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}/\text{GaAs}$ and $\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}/\text{GaAs}/\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}$. Calculation according to formula (3) with parameters from the table.

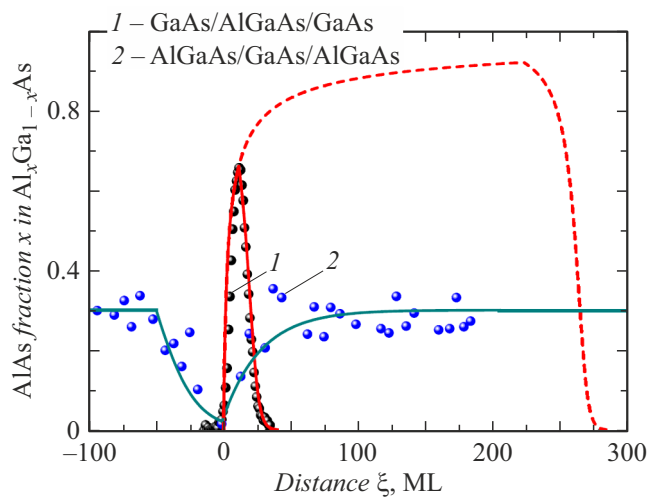


Figure 3. Profiles of composition in double axial heterostructures in selfcatalyzed $\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ [12] and Au- and Au catalyzed NW $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ with initial composition $x_0 = 0.3$ [10](symbols). Lines — show calculation according to formula (3) with parameters from the table.

Parameters of auto- and Au-catalyzed heterostructures in NW AlGaAs

NW/catalyst	T , °C	R , nm	β , deg	$f(\beta)$	χ_{Au}	c_l	F	b	$\Delta\xi$
AlGaAs/Ga	610	60	135	4.28	0	497.0	1480	0.998	2.98
AlGaAs/Au–Ga	510	24	115	10.6	0.5	7.8	237	0.872	15.2

the calculated curves describe the experimental data well. A significant variation of data in Ref. [12] is attributable to the low contrast of GaAs inserts in the body of small-radius GaAs NW. However, it should be noted that the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ inserts in GaAs NW were grown with the Ga flow turned off, i.e. the stationary composition of the inserts is equal to one. Growing the heterostructure to a composition equal to unity would lead to a radical blurring of the interfaces (dashed line in Fig. 3), since the composition with a high content of AlAs requires the displacement of stable Ga atoms from the droplet. It should be noted that obtaining barrier layers of binary AlAs is practically not required. Another difference between the considered NW is that selfcatalyzed NW have a cubic crystal phase [12], while Au-catalytic NW — have a hexagonal phase [9–11]. This fact is not taken into account in the model and requires additional analysis, which will be presented in a separate publication.

Thus, the constructed model is suitable for calculating the composition profiles of axial heterostructures in III–V NW with a liquid–crystal distribution of the form (1). This corresponds to the small lattice mismatch parameters in triple NW based on the mixing of group III atoms, and kinetic composition diagrams in NW based on the mixing of atoms of group V elements. The obtained analytical formula describes well the various experimental data in the AlGaAs system. These results can be used for quantitative analysis and control of the composition of heterostructural NW in a wide range of systems of III–V materials.

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Conflict of interest

The authors declare that they have no conflict of interest.

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