# Quantum wires, quantum dots, and other low-dimensional systems

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## Modeling of interfacial profile of axial GaAs/AlAs nanowire heterostructures

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**Abstract.** We describe the formation of axial GaAs/AlAs heterostructured nanowires grown via the vapor-liquid-solid method. The calculations are based on the combination of mass balance of atoms in the droplet and the nucleation-limited composition of ternary $Al_xGa_{1-x}As$ nanowires. We examine the influence of growth temperature, atomic Al flux and the Au concentration in the liquid on the interfacial abruptness. In particular, we compare the compositional profiles of heterostructures in Au-catalyzed and self-catalyzed nanowires. The obtained results might be useful for growth of GaAs/AlAs heterostructured nanowires.

**Keywords:** interfacial profile, axial heterostructures, AlGaAs, nanowires, modeling

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## Моделирование профиля состава осевой гетероструктуры GaAs/AlAs в нитевидных нанокристаллах

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**Аннотация.** Проведено теоретическое исследование формирования осевой гетероструктуры GaAs/AlAs в нитевидных нанокристаллах, выращенных по механизму пар-жидкость-кристалл. В основе модели лежит материальный баланс в капле, где встраивание атомов в нитевидный нанокристалл лимитировано нуклеацией. Изучено влияние температуры роста, потока алюминия и концентрации золота в капле на резкость гетероперехода. В частности, мы сравниваем профили состава гетероструктурных авто-каталитических и Au-каталитических нитевидных нанокристаллов. Полученные результаты могут быть полезны при росте осевых гетеростуктур GaAs/AlAs в нитевидных нанокристаллах.

**Ключевые слова:** профиль состава, осевые гетероструктуры, AlGaAs, нитевидные нанокристаллы, моделирование

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## Introduction

Semiconductor nanowire heterostructures are one of the most promising nanoscale objects whose properties have attracted much attention from researchers [1]. Axial nanowire heterostructures are usually produced by the so-called vapor-liquid-solid mechanism [2]. A combination of binary compounds provides advanced functionality. Consequently, a wide range of devices based on nanowire heterostructures have been developed, including electronic, photonic and thermoelectric applications [3]. One of the key features of heterostructured nanowires is the heterointerface which determines the quality of optoelectronic applications. Ideally, such nanostructures should be grown with atomic precision which is impossible without understanding the formation mechanism. A particular factor limiting interfacial abruptness is the reservoir effect [4]. Thus, modeling the growth of heterostructured nanowires is of paramount importance. Recent studies [5, 6] have reported on an analytical approach to describing the compositional profiles of axial heterostructures in Au-catalyzed and self-catalyzed nanowires. In this study, we apply our model to a GaAs/AlAs heterojunction and examine the influence of growth temperature, atomic flux of Al and concentration of Au on the interfacial abruptness of heterostructured nanowires grown via the vapor-liquid-solid (VLS) mechanism.

## Materials and Methods

Within the model, we consider VLS growth of an axial nanowire heterostructure from a droplet which initially contains Ga, As, and Au elements (in the case of self-catalyzed growth the Au concentration equals zero). Then we vary the vapor phase composition introducing the flux of Al which makes the droplet quaternary. As a result, an $Al_xGa_{1-x}As$ ternary solid solution forms. It has been shown [6] that the compositional profile across an axial heterostructure can be found from

$$\frac{d\xi}{dx} = \frac{1}{g}\frac{1}{a-x}\frac{dy}{dx}c_{tot}. \quad (1)$$

Here $\xi$ is the axial coordinate across the heterointerface, $x$ is the content of AlAs pairs in the solid, $g$ is the geometrical coefficient, $c_{tot} \approx 1 - c_{Au}$ is the total concentration of group III elements, $a$ is the dimensionless influx of Al, $y = c_{Al} / (c_{Al} + c_{Ga})$ is the liquid composition, $c_{Al}$, $c_{Ga}$, $c_{As}$ and $c_{Au}$ are the concentrations of Al, Ga, As and Au in the droplet, respectively. Eq. (1) is solved by introducing an mechanism to incorporate atoms into the solid, which determines the liquid-solid composition dependence. In our case, we consider the nucleation-limited growth regime which can be applied if supersaturation is low. Then the liquid-solid composition dependence can be written as [7]

$$y = \frac{1}{1 + \frac{1-x}{x}e^{2\omega_{AlAs\text{-}GaAs}(x-1/2)+b}}. \quad (2)$$

Here $\omega_{AlAs\text{-}GaAs}$ is the pseudobinary interaction parameter in the solid and $b$ is a coefficient depending on the As, Ga, Al and Au concentrations in the droplet, the chemical potential differences for the pure components and the interaction parameters in the liquid. All details can be found in [7].

## Results and Discussion

We start to investigate the formation of GaAs/AlAs heterostructured nanowires with analysis of the interfacial profile $x(\xi)$ for different growth temperatures. The values of binary and ternary interaction parameters and Gibbs free energies can be found in [7]. Fig. 1 shows the compositional profile of a GaAs/AlAs nanowire heterostructure at a fixed $c_{Au} = 0$ (self-catalyzed growth), $a = 2$, $g = 0.001$ and $c_{As} = 0.01$. Within the nucleation-limited regime, the compositional control of $Al_xGa_{1-x}As$ nanowires over the entire range is possible at all presented growth temperatures which can be explained by the fact that the AlAs-GaAs pseudobinary interaction parameter has a low enough value. It is seen that the slope of the GaAs/AlAs heterojunction at small and high solid compositions is different (a steep slope at $x < 0.8$ which means that the solid composition changes rapidly with the axial coordinate across the heterointerface (less than 10 monolayers) and a long tail at $x > 0.8$ meaning that a large number of ternary monolayers (~70 monolayers) is needed to achieve the pure AlAs binary). The shape of the $x(\xi)$ curves can be explained by the shape of the liquid-solid composition dependence: a small addition of Al atoms to the droplet leads to a tremendous increase of the Al concentration in the ternary nanowire, except the range of high AlAs content in the solid. Increasing the temperature broadens the heterointerface.

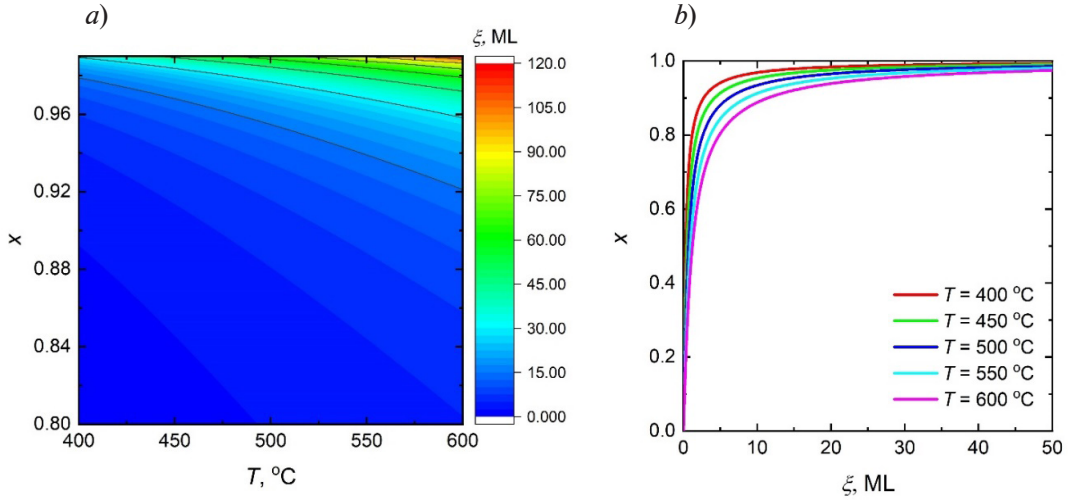


Fig. 1. Contour plot of the GaAs content x in the GaAs/AlAs NW heterostructure NW versus distance ξ and temperature $T$ (*a*); composition profiles $x(\xi)$ across the GaAs/AlAs NW heterostructures at different temperatures $T$ (*b*).

The temperatures $T$ are given in the inset to Fig. 1, *b*. The distance along the nanowire is measured in monolayers (MLs)

Next, we analyze the influence of the concentrations of the foreign catalyst (for the particular case of Au) on the interfacial abruptness of GaAs/AlAs heterostructures. It should be noted that such analysis makes it possible to compare Au-catalyzed and self-catalyzed growth of heterostructured nanowires. The contour plot for variation of the distance ξ with AlAs content $x$ and Au concentration $c_{Au}$ in the GaAs/AlAs nanowire heterostructure and the $x(\xi)$ dependence calculated for different Au concentrations at a fixed $c_{As} = 0.01$, $T = 610$ °C, $a = 2$ and $g = 0.001$ are presented in Fig. 2. Such high temperature might be relevant for GaAs/AlAs heterostructured nanowires [8]. Within the considered range of Au concentrations ($0 < c_{Au} < 0.4$), increasing the Au concentration broadens the heterointerface. However, a heterointerface might be sharper in the case of Au-catalyzed growth as compared to the case of self-catalyzed growth if Au concentration is very high. This is due to the non-monotonic behavior of interfacial abruptness with varying Au concentration. Roughly the same number of monolayers is needed to obtain pure AlAs regardless of Au concentration.

Finally, let us consider the effect of the dimensionless atomic flux on the compositional profile of axial GaAs/AlAs nanowire heterostructures. Fig. 3 shows the contour plot for variation of the distance ξ with AlAs content $x$ and dimensionless atomic flux $a$ in the GaAs/AlAs nanowire heterostructure and the $x(\xi)$ dependence calculated for different dimensionless atomic fluxes at fixed $c_{As} = 0.01$, $T = 610$ °C, $c_{Au} = 0$ and $g = 0.001$. Lower atomic fluxes a result in broader GaAs/AlAs heterointerfaces. This effect is especially crucial when $a$ tends to 1.

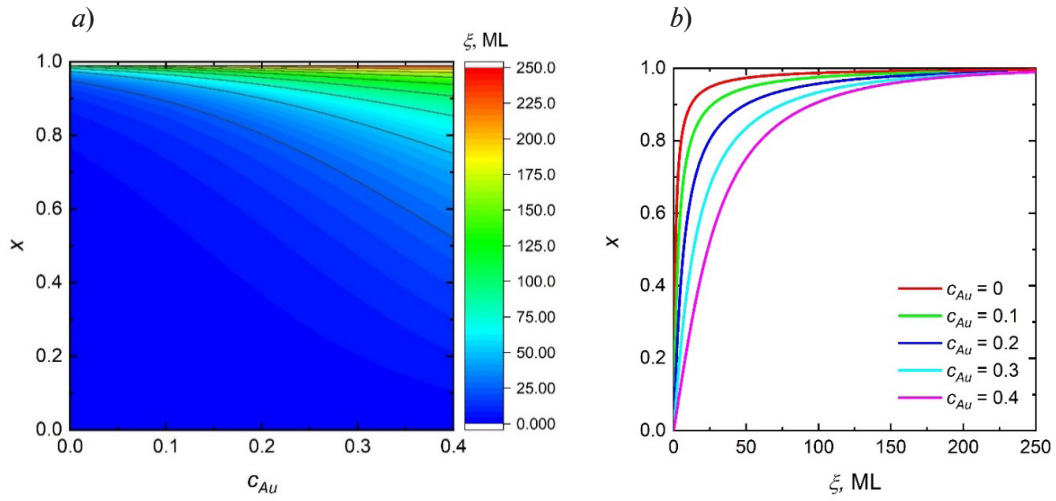


Fig. 2. Contour plot of the GaAs content x in the GaAs/AlAs NW heterostructure NW versus distance ξ and Au concentration $c_{Au}$ (*a*);composition profiles $x(\xi)$ across the GaAs/AlAs NW heterostructures at different Au concentrations $c_{Au}$ in the droplet (*b*).
The concentrations $c_{Au}$ are given in the inset to Fig. 2, *b*

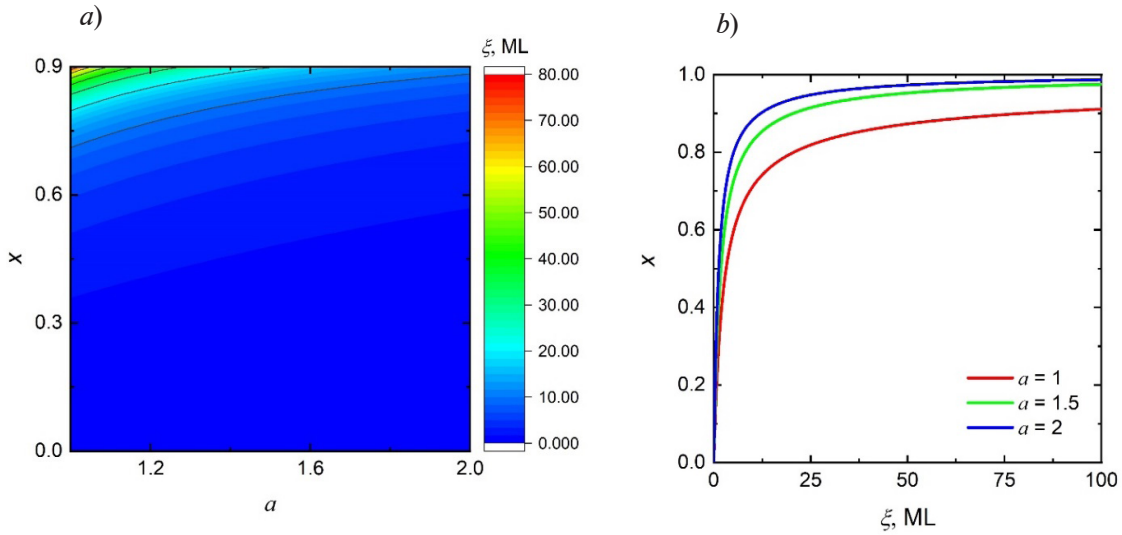


Fig. 3. Contour plot of the GaAs content *x* in the InAs/GaAs NW heterostructure NW versus distance ξ and dimensionless atomic flux *a* (*a*); composition profiles $x(\xi)$ across the GaAs/AlAs NW heterostructures at different dimensionless atomic fluxes *a* (*b*).
The dimensionless atomic fluxes a are given in the inset to Fig. 3, *b*

## Conclusion

To summarize, we have calculated the interfacial profiles of axial GaAs/AlAs heterostructures in self-catalyzed and Au-catalyzed nanowires grown in the nucleation-limited regime. Special attention is paid to the influence of the concentrations of the foreign catalyst (on the example of gold), temperature and atomic flux on the interfacial abruptness of GaAs/AlAs heterostructures. Our findings confirm that decreasing the growth temperature and Au concentration and increasing the atomic flux can improve the interface abruptness of the GaAs/AlAs heterojunction. The obtained results may be useful for growth of GaAs/AlAs heterostructured nanowires.

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