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Nanostructures Nucleation Features and Miscibility Analysis in Zinc-Blend and Wurtzite GaN-InN-AlN Material System

A.K. Simonya, K.M. Gambaryan*, V.M. Aroutiounian

Department of Physics of Semiconductors and Microelectronics, Yerevan State University, Yerevan – 0025, Armenia.

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ABSTRACT

The growth mechanism of quantum dots (QDs) and nanopits in GaN-InN-AlN material system for both zinc-blend and wurtzite structures is theoretically investigated. The continuum elasticity model is used for calculations. The nanostructures energy versus their volume, as well as the critical energy and critical volume versus the QD and wetting layer lattice constants relative mismatch ratio (strain ε), are calculated. It was shown that when the zinc-blend GaN is used as a substrate and when the strain between the wetting layer and a substrate overcomes critical ε^*=0.039 value, instead of QDs nucleation, the formation of nanopits becomes energetically preferable. Otherwise, when wurtzite GaN is used as a substrate the critical strain is equal to ε^*=0.01, i.e. almost four times smaller. Miscibility gap analysis for GaInAlN quaternary material system is performed by the Gibbs free energy calculations. It is shown that immiscibility gap strongly depends not only on temperature, but also on crystallographic structure. Presented results can be useful at QDs engineering, as well as at the growth of multicomponent bulk crystals and epitaxial thin films in GaInAlN material system.

1. Introduction

The quantum dots (QDs) and other nanostructures, along with the choosing of corresponding advanced semiconducting materials and their band gap engineering, open up entirely new functionalities of traditional devices as well as new challenges for the fabrication of devices with unique properties. In particularly, single photon sources for quantum cryptography, QD lasers, single photon detectors, single electron transistors, resonant tunneling diodes, etc [1-4]. Indeed, the physical properties of QDs depend on QDs size and shape, as well as on the mechanism of their formation. The most useful approach for the fabrication of QDs is Stranski–Krastanov [5] growth mode, where the sum of the surface free energy and the interface free energy is about the same as the substrate free energy. In this case, the wetting layer is compressively strained in a few percent. Interestingly note that in the original publication by Stranski and Krastanov, no strain effects were considered. The strain relaxation leads to the formation of coherent (dislocation free) islands on top of a thin wetting layer. Depending on the strain value and its sign, the growth of QDs, the formation of nanopits or even QDs–nanopits cooperative structure can be achieved.

Binary III-V compound semiconductors, especially nitrides and their ternary and quaternary alloys are very attractive for several applications [6]. For instance, GaInN alloys are used for fabrication of blue and green light emitted diodes, as well as for violet and blue lasers [7]. Since the band gap of GaInN can be varied from 2.0 to 3.5 eV by increasing of GaN concentration, the potential operating wavelengths cover nearly the entire visible spectra range [8, 9]. High-speed field effect transistors, high-temperature electronic devices, UV and blue light emitters, detectors and gas sensors were made of GaN [10]. Among III-nitride semiconductors, InN has the lowest effective mass and small band gap. Therefore, InN-related solid solutions can extend the emission or absorption from the UV to near infrared regions. The photovoltaic (PV) and thermo-PV cells were also fabricated using InN [10].

While zinc-blend film/zinc-blend substrate combinations have been analyzed previously [11], systems involving hexagonally oriented material as either the film or substrate have not been thoroughly investigated. Examples of important semiconductor materials that exist in the hexagonal crystal structure include the wide bandgap compound semiconductors GaN, SiC and many II–VI semiconductors. The growth of hexagonal materials has been extensively studied experimentally, however, quantitative calculation of the inherent strain energy has not been fully performed. Furthermore, the effect of the strain energy on the resulting equilibrium has not been addressed. In [12], elastic compliance equations are developed and their relationship to the overall strain energy of a hexagonally oriented film and substrate are presented. These general relations are then applied to the growth of GaN on different substrates. Additionally, the sufficient lattice mismatch between the III-N binary compounds allows growing of nanostructures in Stranski–Krastanov growth mode.

Regarding the research and development of III-nitride QDs, there are three main kinds of formation mechanism for the growth of QDs. First, it has been proposed [13] that nanoscale indium composition fluctuation due to InGaN phase separation or indium segregation results in the formation of indium-rich clusters, which acts as QDs (QDs-like). Hence, QDs-like system acts as an extremely sophisticated quantum capture system, and in QDs, the charge carriers are deeply localized so as to hinder their migration toward nonradiative defects (dislocations). Therefore, high luminescence efficiency could be expected if the density of QDs is much higher than that of dislocations. Second, it has been shown that nitride QDs can be self-organized using the strain-induced Stranski-Krastanov growth mode [14]. Third, another way to form nitride QDs is to take advantage of surfactants or antisurfactants, which are often used to change the surface free energy of heterostructure interface. However, the self-assembled nitride QDs can be fabricated by molecular-beam epitaxy or by metalorganic chemical vapor deposition [13, 14] without using any antisurfactants. High-density GaN/AlN QDs for deep UV LED with high quantum efficiency [15] have been also successfully grown by molecular beam epitaxy.

In this paper, the competing growth mechanism of QDs or nanopits in GaN-InN-AlN material system both for zinc-blend and wurtzite configurations is theoretically investigated using the continuum elasticity model proposed by J. Tersoff (IBM) [1, 16]. Additionally, miscibility gap analysis for the GaInAlN quaternary material system is performed by the Gibbs free energy calculations.

*Corresponding Author
Email Address: kgambaryan@ysu.am (K.M. Gambaryan)

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