Physical Vapor Transport Growth of bulk $Al_{1-x}Sc_xN$ Single Crystals

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1. Introduction

Development of semiconductor light sources operating in the ultraviolet (UV) range, such as UV light-emitting diodes (LEDs) and laser diodes (LDs) are in the focus of current research, with technological applications in mind such as sterilization, purification of water and air, medical treatment of skin diseases, promotion of plant growth, physico-chemical analysis of surfaces and particles, and much more [1,2]. The respective devices consist of ternary AlGaN and quaternary InAlGaN thin films [3], as these compounds can cover the band-gap region between 6.0 eV (AlN) and 3.4 eV (GaN), i.e. 210 nm to 360 nm emission wavelength, by forming solid solutions. The external quantum efficiencies (EQE) are found to decrease with decreasing emission wavelength mainly because of charge carrier injection and transport in films with higher Al content, in particular for Al concentrations higher than 70 at. % at [3]. On the other hand, EQE values exceeding 10 % for 280 nm LEDs [4] have been recently achieved as the corresponding strained thin films can be coherently grown on AlN templates or bulk single crystals [5], which limits the generation of dislocations in the active layers. In contrast to that, AlGaN based UVB LEDs with emission wavelengths of about 300 nm still suffer from relatively low EQEs of around 2 % and emission powers in the µW range [4]. The main reason for this problem is the lack of lattice-matched substrates. As a result, such layers exhibit threading dislocation densities (TDD) > 10^9 cm^{-2} in the active layers, while TDD < 10^6 cm^{-2} would be desirable [6].

Recently, theoretical investigations by Moram and coworkers [7,8] consider the replacement of Al in AlN by transition metals with an oxidation state of +3. Scandium in the state +3 exhibits a larger ionic radius than any other 4th raw transition metal in the +3 state and, hence, it might be expected that $Al_{1-x}Sc_xN$ is less stable than other transition metal nitrides (TMNs)-alloys. However, electronic effects associated with the Sc 3d orbitals have to be considered as well. These orbitals contributing to the conduction band are empty and the Fermi level is located inside the band gap. This leads to a greater relative stabilization of the wurtzite phase for $Al_{1-x}Sc_xN$ than for other TMN-alloys at equal TMNs concentrations. The same authorshave predicted that $Al_{1-x}Sc_xN$ substrates with $x \approx 0.08$ exhibit lattice parameter matching to $Al_{0.5}Ga_{0.5}N$. The latter composition is needed for devices emitting at about 300 nm. As experiments have shown [5] that the critical thickness for plastic relaxation (as the limit for pseudomorphically strained layers) exceeds 1 µm for $Al_{0.7}Ga_{0.3}N$ on AlN substrates, some residual compressive stress is allowed in the system before relaxation leads to generation of dislocations. Thus,