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Mid-Infrared Ellipsometry, Raman and X-ray Diffraction Studies of $Al_xGa_{1-x}N$/AlN/Si Structures

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Abstract

We report an investigation of the optical and structural properties of wurtzite phase $Al_xGa_{1-x}N$/AlN structure grown on Si(111) within the compositional range of $0 \leq x \leq 1$. The study focuses on providing essential physical quantities for the fabrication process control, namely the composition dependence of phonon mode energy and refractive index. Three complementary techniques, infrared ellipsometry, Raman spectroscopy and X-ray diffraction, have been used to minimize uncertainties in our analysis. Based on the high quality and nearly strain-free $Al_xGa_{1-x}N$/AlN double layer samples, we determined the calibration curve for the A_1(LO) phonon mode. We have also constructed the ellipsometry model which uses *a-priori* knowledge of experimentally measured A_1(TO) phonon mode frequencies. From the best model fit to the collected ellipsometry spectra of the entire sample series, we obtained the anisotropic refractive indices of the $Al_xGa_{1-x}N$ alloys with a very satisfactory accuracy.

I. Introduction

The group III nitrides and their heterostructures are technologically important in optoelectric, high power and high frequency electronic devices, owing to the materials' wide tunable bandgap [1] and the ability of formation a two-dimensional electron gas with high sheet charge carrier density [2]. The fabrication of group III nitride devices can use sapphire, silicon-carbide or silicon substrates [3]. Among them silicon substrate attracts considerable attention due to the potential of bringing down the fabrication cost, by using less expensive material and boosting the production volume with large diameter wafers.

The well known obstacle in fabrication of high-quality layers is the lattice mismatch between the nitrides and the silicon substrate, as well as the difference in their thermal expansion coefficients. The problem causes phase separation and high defect density in the epitaxial layers, which makes the quality of the GaN epitaxial layer by direct growth on silicon far from satisfactory. In order to overcome this problem, an alternative approach of introducing an interlayer, like (HT)AlN-Si [4], (LT)AlN-(HT)AlN-Si [5],