

Microstructure of $\text{GaN}_{1-x}\text{Bi}_x$

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In this paper we describe detailed transmission electron microscopy studies of $\text{GaN}_{1-x}\text{Bi}_x$ with $0.05 < x < 0.18$ grown by low-temperature molecular beam epitaxy under Ga-rich conditions. Microstructural transformation from columnar growth separated by thin amorphous areas in the films with lowest Bi content (5%) to pseudo-amorphous structure with crystalline grains embedded in the amorphous matrix in the samples with higher Bi content (13% to 18%) was observed. In addition, metallic Bi segregation occurred in the samples with the highest Bi concentration. An abrupt decrease in absorption edge energy is found in samples with higher Bi content.

Key words: Microstructure, TEM, GaNBi, highly mismatched semiconductors, absorption, bandgap

INTRODUCTION

Development of high-efficiency multijunction solar cells with multilayers of materials with different bandgaps is always challenging due to the limited availability of materials with suitable bandgaps to cover the entire solar spectrum. Typically the various subcells in a multijunction device with different bandgaps are grown epitaxially on top of each other. In these structures, lattice matching between each layer of different material is required to avoid high defect density at the various interfaces that may be detrimental to device performance (see, for example, the review by Coatal et al.¹). Therefore, there is a constant search for new materials which would absorb the whole solar spectrum but would not easily form structural defects that will affect carrier transport. In our recent report using highly non-equilibrium low-temperature molecular beam epitaxy (LT-MBE) we demonstrated the synthesis of highly mismatched $\text{GaN}_{1-x}\text{As}_x$ alloys in the full composition range and showed that the optical bandgap decreases monotonically with increasing As concentration.^{2,3} Continuous change of the bandgap

was observed even though the films with $0.1 < x < 0.75$ were amorphous. The amorphous nature of these alloys can be advantageous since no lattice matching is required when alloys with different compositions are used for multijunction solar cells. This successful synthesis of highly mismatched $\text{GaN}_{1-x}\text{As}_x$ alloys suggested that synthesis of other III-V highly mismatched alloys with electronic structure and optical properties suitable for photovoltaic applications may also be possible using similar techniques. This paper reports on our investigation on $\text{GaAs}_{1-x}\text{Bi}_x$, an alloy system that has anion mismatch much stronger than in $\text{GaN}_{1-x}\text{As}_x$.

Recently, it was reported that it is possible to grow highly mismatched $\text{GaAs}_{1-x}\text{Bi}_x$ alloys with limited Bi content with dramatic modifications in the electronic band structures by both metalorganic vapor-phase epitaxy (MOVPE) and molecular beam epitaxy (MBE).^{4–8} We realize that incorporation of Bi into GaN is more difficult than incorporation of As into GaN because of the extremely large differences between Bi and N in terms of electronegativity (1.8 eV and 3.0 eV) and atomic radius (155 pm and 75 pm). Also, GaBi binary compound has never been grown and only a theoretical negative bandgap value for GaBi has been reported.⁶ Using the LT-MBE method, we recently reported synthesis of

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