分子束磊晶成長的三元合金氧化鎂鋅之應力效應分析

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摘 要

三元合金氧化鎂鋅是屬於一種極具潛力的寬帶半導體材料，因爲此材料可藉由調節鋅（Zn）或鎂（Mg）的含量來改變其能帶隙和晶格參數以達到短波長光子元件的應用，例如: 紫外線偵測器、發光二極體與雷射二極體。目前我們努力的目標是將可控制的不同鎂含量的氧化鎂鋅以分子束磊晶法成長在三氧化二鋁的基板上。爲了分析鎂在晶格中的影響，我們必須探討到此元素在氧化鎂鋅中會造成壓縮或拉伸應變效應。因此，X光繞射會用來量測氧化鎂鋅樣品。詳細的實驗步驟與數據分析將會被比較和討論。

關鍵詞：氧化鎂鋅，應力，X光繞射

Characterization of strain effects of ZnMgO ternary alloys grown by MBE

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ABSTRACT

Ternary alloys of ZnMgO have been proposed as the promising wide band semiconductor materials due to the adjustable band gap and lattice parameter by varying zinc (Zn) and/or magnesium (Mg) compositions for the application of the short-wavelength photonic devices such as ultraviolet detectors, light-emitting diodes, and laser diodes. Our current effort in investigating the strain effects of $Zn_{1-x}Mg_xO$ materials has been implemented by producing the samples on the Al_2O_3 substrates with different controlled level of Mg compositions by the Molecular Beam Epitaxy (MBE) method. To analyze the effect of the incorporation of Mg in the lattice, we must take into account that the $Zn_{1-x}Mg_xO$ layer is under compressive or tensile strain depending on its composition. Then, $Zn_{1-x}Mg_xO$ samples can be assessed by the measurements of X-ray diffraction (XRD). The detailed experiment procedure and explanation are compared and discussed.

Key Words: ZnMgO, Strain, XRD

1. Introduction

Ternary alloys of ZnMgO have been proposed as the promising wide band semiconductor materials due to the adjustable band gap and lattice parameter by varying zinc (Zn) and/or magnesium (Mg) compositions for the application of the short-wavelength photonic devices such as ultraviolet detectors, light-emitting diodes, and laser diodes [1-3]. Despite their various technological applications, the theoretical and experimental understanding of the solid-state properties of various Mg contents in ZnMgO is still relatively incomplete. In this work, we report the strain effects of ZnMgO films produced via the molecular beam epitaxy (MBE) on the sapphire substrate.

2. Experimental

$Zn_{1-x}Mg_xO$ materials have been implemented by producing the samples on the Al_2O_3 substrates with different controlled level of the Mg compositions by plasma-assisted molecular beam epitaxy (PA-MBE) method. Each sample was grown on the first buffer layer of ZnO and second buffer layer of MgO at the substrate temperature of 650 °C. During the processing of sample preparations, the Mg flux was in the range of 5.52×10^{-9} – 2.05×10^{-8} Torr. The compositions of the $Zn_{1-x}Mg_xO$ samples were identified by Energy-dispersive X-ray spectroscopy (EDX), and the Mg (Magnesium) content in each of the three samples was estimated to be 3.3% for #51, 6.4% for #48, and 8.3% for #46, respectively. The strain effects of the $Zn_{1-x}Mg_xO$ heterostructure ternary alloys were analyzed by means of the X-ray diffraction (XRD) method.

3. Results and discussion

In order to investigate the effects of different Mg contents of ZnMgO ternary alloys, it is quite necessary to analyze the influence of the incorporation of Mg in the lattice. To examine the effect of Mg incorporation in the lattice, we might take into account that the ZnMgO layer is under compressive or tensile strain depending on its composition. Then, the crystal structure and orientation were investigated by the XRD measurements of

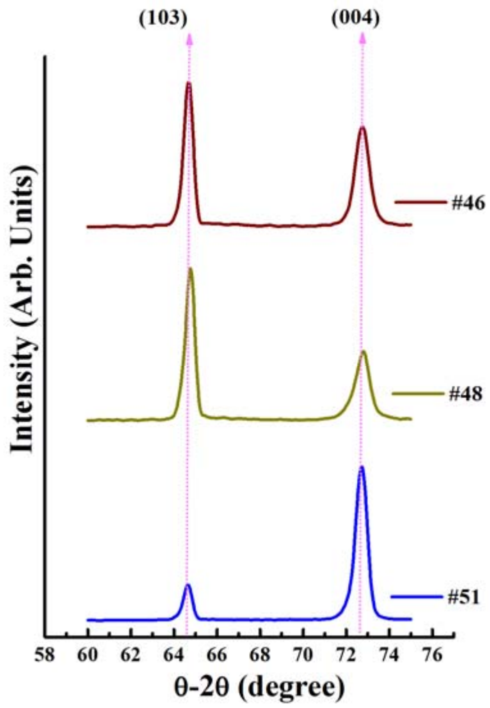

Fig. 1 XRD spectra in the range of 60 - 75° are shown here, it is found that all the samples show preferred orientations of (004) to characterize the hexagonal wurtzite structure with the strongly *c*-axis oriented but the peak of (103) is from the sapphire substrate

θ - 2θ scan in the range of 60 - 75°. As shown in Fig. 1, it is found that all the samples show preferred orientations of (004) to characterize the hexagonal wurtzite structure with the strongly *c*-axis oriented but the peak of (103) is from the sapphire substrate [2]. This points out that the *c*-axis of the grains becomes uniformly perpendicular to the sapphire substrate surface, indicating the formation of ZnMgO alloys with wurtzite structure. In order to study the influence of Mg content in the ZnO material, we would like to pay our attention to the peak position of (004). The shifting of (004) peak is directly related to '*c*' axis length and calculated by using the Bragg's law for the (004) plane by $c = \lambda/\sin\theta$, where λ and θ are the x-ray wavelength and the diffraction angle of the epitaxial layers, respectively [4]. As a result, the *c*-axis length monotonically reduced from 5.196 Å (x = 3.3%) to 5.185 Å (x

= 8.3%) and this reduction in the '*c*' axis length could be explained with the fact that in the ZnMgO hexagonal lattice, part of Zn^{2+} (0.60 Å) ions are replaced by somewhat smaller Mg^{2+} (0.57 Å) ions [5]. Probably, as more Mg was introduced into the sample, Mg embedded itself in an interstitial position, which leads to a decrease of the lattice constants.

As we have known that the variation of residual stress might influence the lattice constant "*c*" of ZnMgO films, so we specifically investigate the residual stress in ZnMgO samples by considering the (004) peaks in XRD spectra. The lattice constant can be further utilized to evaluate the average uniform strain, σs in the lattice along the *c*-axis can defined as: $\sigma_s = \frac{2c_{13}^2 - c_{33}(c_{11}+c_{12})}{2c_{13}} \times \frac{c-c_0}{c_0}$ where c_{ij} (i, j = 1, 2, 3) stands for the elastic constants in different orientation; c_0 is the lattice constant of ZnO (5.205 Å), and *c* is the lattice constant of our ZnMgO sample [6]. Then, the residual stress σs in those ZnMgO samples can be obtained by substituting the value of c_{ij} (i, j = 1, 2, 3) in the above equation with c_{11} = 207.0 GPa, c_{12} = 117.7 GPa, c13 = 106.1 GPa, and c_{33} = 209.5 GPa, respectively [6]. The calculated results are determined to be 0.427 GPa for #51, 0.528 GPa for #48, and 0.882 GPa for #46, respectively. The stress is positive to indicate that the biaxial stress is tensile and the residual stress of the ZnMgO samples was increased as the Mg content was increased [7]. Then the results of residual stress are quite confirmed as the Mg composition increased, the ZnMgO (004) diffraction peaks approaching the higher degree side.

4. Conclusions

The ternary alloys in the structure containing ZnMgO film with different Mg contents have been investigated by the XRD techniques. Furthermore, the higher Mg contents samples contributing to the larger values of stress. As a result, it is interesting to notice that structural property is more strongly influenced by the fact of Mg in the Zn-Mg-O alloy system.

Acknowledgement

The authors would like to acknowledge the support of the National Science Council Project NSC102-2221-E-272-006 and NSC99-2112-M-236-001-MY3.

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