



Microstructural and surface property variations due to the amorphous region formed by thermal annealing in Al-doped ZnO thin films grown on n-Si (1 0 0) substrates

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ABSTRACT

X-ray diffraction (XRD) patterns revealed that the as-grown and annealed Al-doped ZnO (AZO) films grown on the n-Si (1 0 0) substrates were polycrystalline. Transmission electron microscopy (TEM) images showed that bright-contrast regions existed in the grain boundary, and high-resolution TEM (HRTEM) images showed that the bright-contrast regions with an amorphous phase were embedded in the ZnO grains. While the surface roughness of the AZO film annealed at 800 °C became smoother, those of the AZO films annealed at 900 and 1000 °C became rougher. XRD patterns, TEM images, selected-area electron diffraction patterns, HRTEM images, and atomic force microscopy (AFM) images showed that the crystallinity in the AZO thin films grown on the n-Si (1 0 0) substrates was enhanced resulting from the release in the strain energy for the AZO thin films due to thermal annealing at 800 °C. XRD patterns and AFM images show that the crystallinity of the AZO thin films annealed at 1000 °C deteriorated due to the formation of the amorphous phase in the ZnO thin films.

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1. Introduction

ZnO wide gap semiconductors have attracted a great deal of current interest because of their promising applications in optoelectronic devices, such as ultraviolet laser diodes [1], light emitting diodes [2], photodetectors [3], surface acoustic wave devices [4], and thin film transistors [5]. The prospect of potential applications of optoelectronic devices utilizing ZnO semiconductors has led to substantial research and development efforts to form various types of ZnO materials on several substrates [1–5]. Because ZnO thin films have peculiar physical properties, such as low dielectric constants, high chemical stabilizations, large bond strengths, large exciton binding energies, and good photoelectric and piezoelectric properties, in comparison with GaN-based materials [6–8], they have promising advantages for applications in short-wavelength devices. The group III element, such as Al, Ga, or In, doped ZnO thin films have emerged as excellent candidates for potential applications as transparent electrodes in optoelec-

tronic devices. However, because the dopants typically have a large affinity with O₂ atoms rather than Zn atoms during the growth processes of the doped ZnO, faulted oxide results, which degrades the physical properties of the thin films. The electrical and optical properties of doped ZnO can be improved by post-annealing treatment [9–11]. Among the various types of doped ZnO thin films, Al-doped ZnO (AZO) thin films have attracted a great deal of interest from suitable electrodes because ZnO thin films are more stable in a reductive ambient atmosphere, have a more abundant supply, and a lower cost in comparison with indium–tin-oxide films which make them appropriate for potential use as anodes in organic light-emitting diodes [12–16]. While the electrical resistivity of the AZO thin films dramatically decreases in comparison with that of ZnO thin films, high optical transparency in the visible spectral range remains. Because the electrical and optical properties of AZO thin films are significantly affected by their microstructural properties, studies concerning the microstructural property variations due to the amorphous region formed by thermal annealing in the AZO thin films grown on n-Si (1 0 0) substrates are very important for improving the efficiencies of optoelectronic devices fabricated utilizing ZnO/Si heterostructures.

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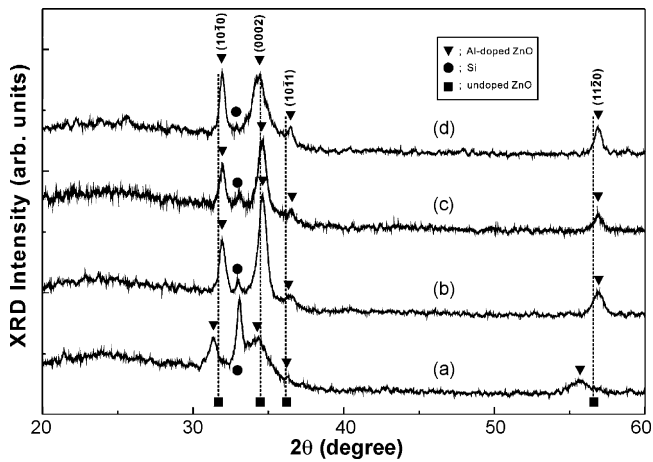


Fig. 1. X-ray diffraction patterns of (a) as-grown Al-doped ZnO thin films grown on n-Si (1 0 0) substrates and of those annealed for 10 min at (b) 800, (c) 900, and (d) 1000 °C. Filled squares represent the (10 $\bar{1}$ 0), (0002), (10 $\bar{1}$ 1), and (11 $\bar{2}$ 0) diffraction peaks corresponding to the undoped ZnO film.

This paper reports data on the microstructural property variations due to the amorphous region formed by thermal annealing in the AZO thin films grown on n-Si (1 0 0) substrates by using radio-frequency magnetron sputtering. X-ray diffraction

Table 1

Strains of (10 $\bar{1}$ 0), (0002), (10 $\bar{1}$ 1), and (11 $\bar{2}$ 0) planes for the as-grown AZO thin film and for those annealed at 800, 900, and 1000 °C, as determined from the XRD data.

Strain (%); plane	Annealing temperature (°C)			
	As-grown	800	900	1000
(10 $\bar{1}$ 0)	1.75	-0.15	-0.15	0.06
(0002)	-0.16	-0.13	0.16	0.29
(10 $\bar{1}$ 1)	0.44	0.14	-0.07	-0.07
(11 $\bar{2}$ 0)	1.86	-0.23	-0.22	-0.12

(XRD) measurements were carried out to investigate the crystallization of the AZO thin film, and transmission electron microscopy (TEM) and selected-area electron diffraction (SAED) patterns were obtained in order to investigate the microstructural properties of the ZnO/n-Si (1 0 0) heterostructures. Atomic force microscopy (AFM) measurements were performed in order to characterize the surface smoothness of the AZO thin films. The amorphous phase formation process and mechanism of the ZnO thin film due to the thermal annealing are described on the basis of the TEM and the SAED results.

2. Experimental details

The AZO thin films used in this study were prepared on P-doped n-Si (1 0 0) substrates by using radio-frequency magnetron sputtering. Polycrystalline stoichiometric 2 wt% Al₂O₃-doped ZnO

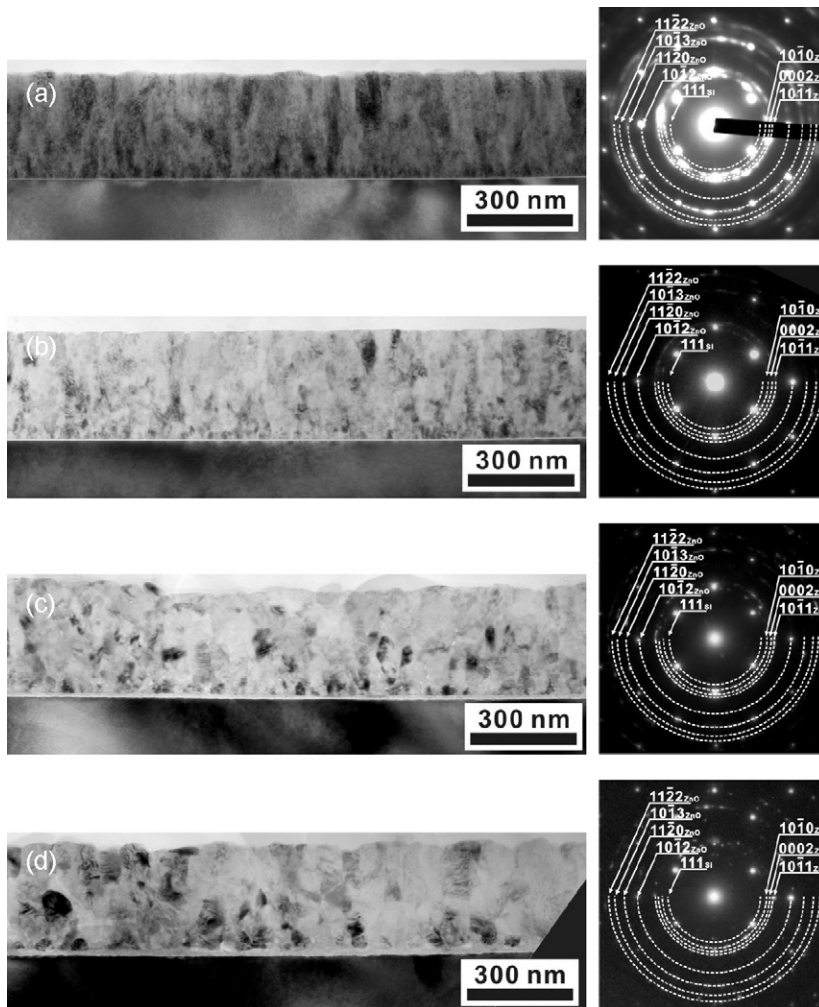


Fig. 2. (a) Cross-sectional TEM images and corresponding SAED patterns of the Al-doped ZnO films annealed at (b) 800, (c) 900, and (d) 1000 °C, along with the [1 1 0] zone axis of the Si substrate.

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