ELSEVIER

Materials Characterization 58 (2007) 750 – 755

MATERIALS CHARACTERIZATION

Microstructural characterization of textured ZnS thin films

T. Kryshtab *, J.A. Andraca-Adame, A. Kryvko

Instituto Politécnico Nacional-Escuela Superior de Física y Matemáticas, Av. IPN, Ed. 9, U.P.A.L.M., 07738, Mexico D.F., Mexico

Received 12 June 2006; received in revised form 6 October 2006; accepted 16 November 2006

Abstract

During thin film growth texture formation is controlled by several kinetic parameters that determine the grain structural evolution. For highly textured thin films, i.e. only one strong peak can be obtained from X-ray diffraction pattern, it is impossible to separate the effect of grain size and residual strains based on peak broadening. We propose an original method for evaluating residual strains, eliminating their contribution in peak breadth and determining the domain size. A two-axes diffractometer with a Ge monochromator and a $K_{\alpha 1,2}$ doublet was used for this study. The measurements of 2θ scans were carried out in the grazing geometry for the incident beam. ZnS thin films as-deposited and annealed were studied. Structural analysis was carried out using a one-axis diffractometer for a θ–2θ scan in the standard symmetric geometry. Surface morphology was explored by atomic force microscopy. The specification of the proposed method and its application in microstructural characterization are introduced.
© 2006 Elsevier Inc. All rights reserved.

Keywords: Thin film; X-ray diffraction; Strains; Domain size

1. Introduction

Thin films are important for a variety of applications, for example, optoelectronic devices. The deposition of polycrystalline thin films is a highly dynamic process carried out far from equilibrium. Textural and microstructural formations depend on a wide range of controllable and uncontrollable variables, which prevents a prediction of the texture and microstructure. However, the optical and electrical properties of devices strongly depend on the thin film microstructure. Characterization of the microstructure is a prerequisite for understanding the growth process and the behavior of thin films.

The study of microstructural features of materials by means of the X-ray diffraction (XRD) line profile analysis is based on a simple model, which says that dislocations in a polycrystalline material subdivide the original grains into small coherent domains and produce tensile or compressive strains within the domains. Both these factors result in broadening of XRD peaks. A well-known approach of Warren and Averbach [1,2] is used to separate the contributions of domain size and strains into the broadening of XRD lines. In later publications [3–5] a development of this method for analysis of XRD line broadening was proposed. The main conception for the separation of their contributions in XRD line breadth is based on the different dependences of XRD line broadening on diffraction angle for domain size and for residual strains. Therefore a set of XRD lines should be used for the determination of microstructural parameters. For highly textured thin films, sometimes only one strong peak can be observed in the XRD pattern and the

* Corresponding author. ESFM-IPN, Av. IPN, Unidad “A.L.M.”, Edificio 9, Col. Lindavista, c.p. 07738, México D.F., México. Tel.: +52 55 5729 6000x55321; fax: +52 55 5586 2825.
E-mail address: tkrysh@esfm.ipn.mx (T. Kryshtab).

1044-5803/$ - see front matter © 2006 Elsevier Inc. All rights reserved.
doi:10.1016/j.matchar.2006.11.011

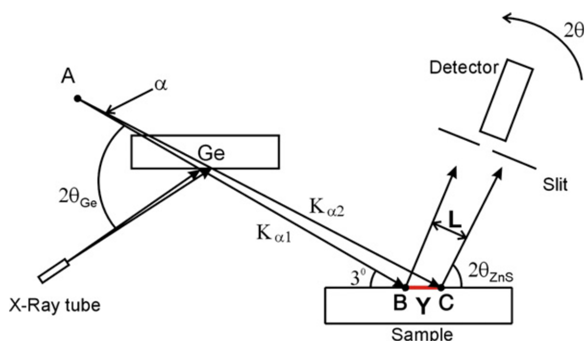

Fig. 1. A schematic of the grazing geometry for a Cu $K_{\alpha1,2}$ doublet after the 220 reflection from a Ge monochromator.

other peaks are very weak and fuzzy and/or overlap with the peaks from the substrate. In this case the separation of the effects of domain size and residual strains on the XRD line broadening and their accurate determination is impossible.

In this study an original XRD method for the determination of domain size and residual strains in textured thin films using one XRD line is proposed. This method gives the possibility of evaluating the strains in thin films, eliminating their contributions to the peak breadth and therefore accurately determining the domain size.

2. Experimental methods

To investigate the residual strains and domain size in textured ZnS thin films an original XRD method is developed. A two-axes diffractometer (DRON-3) with a plane Ge monochromator (220 reflection) was used. The measurements were carried out in the asymmetric grazing geometry for an incident beam containing the Cu $K_{\alpha1,2}$ doublet. A schematic of the peak profile measurement is illustrated in Fig. 1.

A ZnS thin film sample with a polycrystalline structure is placed in a fixed position at an angle of 3° with respect to the incident beam. After reflection from the Ge monochromator two beams of the Cu $K_{\alpha1,2}$ doublet ($K_{\alpha1}$=0.1540 nm, $K_{\alpha2}$=0.1544 nm) will reach the sample at two points B and C. In the case of a flat surface sample the distance Y between these points can be calculated from the geometric factors presented in Fig. 1. The value of Y is 6.02 mm in the case where the distance from the X-ray tube to the sample (the goniometer radius) is 300 mm and the difference in the diffraction angles $\theta_{K\alpha1}$ and $\theta_{K\alpha2}$ for the Ge monochromator α=0.059°. The distance between the two beams of the $K_{\alpha1,2}$ doublet reflected from the ZnS thin film with the 111 reflection L will be equal to 2.59 mm without taking into account the divergence of the doublet beams due to the diffraction from polycrystalline ZnS. Forasmuch as the detector measures the peak positions for $K_{\alpha1}$ and $K_{\alpha2}$ reflections in angles, the spacing between the peaks is 0.495°. Taking into account the divergence of the two reflected beams with two wavelengths of the $K_{\alpha1,2}$ doublet, the spacing between these peaks for a flat sample with the ZnS thin film $\Delta\theta_{cal}$ is equal to 0.535°. This spacing also can be determined from the XRD line profile, measured from a standard sample in the same grazing geometry (a ZnS annealed powder sample with a flat surface) and fitted with some analytic functions taking into account that the observed line profile is the diffraction line with the $K_{\alpha1,2}$ doublet.

The presence of residual strains in a thin film leads to a curving of the sample, concave for a tensile-stressed film and convex for a compressed one. The values of residual stresses and deformation in thin films can be determined from the bending of the samples. The radius of curvature R is calculated from the difference of the interbeam spacing between the peak positions for the reflected $K_{\alpha1,2}$ doublet $\Delta\theta_{meas}$ and the calculated one $\Delta\theta_{cal}$. Taking into account the small value of this

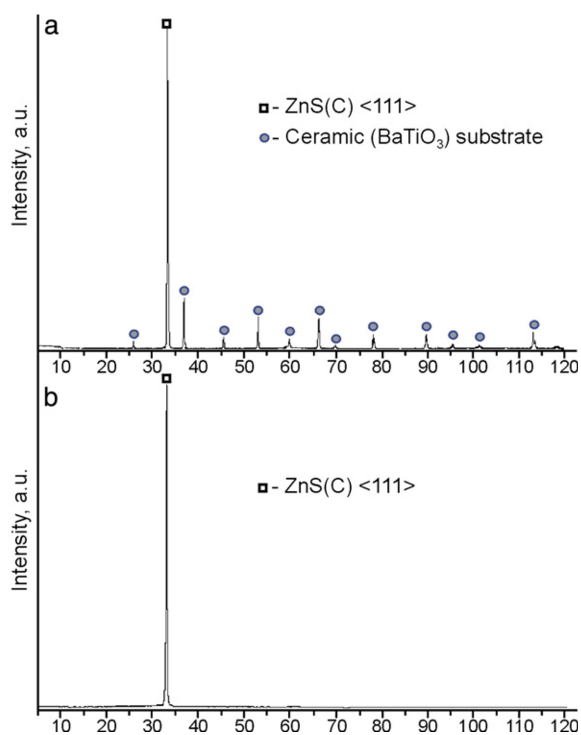

Fig. 2. XRD patterns of ZnS thin films deposited onto ceramic (a) and glass (b) substrates, respectively.

Download English Version:

https://daneshyari.com/en/article/1572438

Download Persian Version:

https://daneshyari.com/article/1572438

Daneshyari.com