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<AT>Evolution of Al:ZnO optical response as a function of doping level

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<ABS-HEAD>Highlights► ZnO and Al:ZnO have been deposited with Al concentration in the range of 0 - 4.2%. ► The Tanguy based model effectively describes the dielectric function evolution. ► There is a correlation between layer optical properties and surface morphology. ► ρ_{opt} derived from Drude model shows a parabolic dependence with Al concentration.

<ABS-HEAD>Abstract

<ABS-P>ZnO and Al doped ZnO thin layers (<100 nm) have been deposited through RF magnetron sputtering on quartz and Si substrates. Structural (XRD), compositional (SNMS), morphological (SEM) and optical/electrical (Spectroscopical Ellipsomtery) characteristics of the samples have been studied in order to deduct the effect of dopant level variation. A combination of classical Tanguy+Drude+Sellmeier terms are used to analyze the dielectric function of ZnO and Al:ZnO. It has been found that increasing Al contents leads to smaller crystalline size, band gap shift and a gradual reduction of the refractive index and increase of the broadening of this transition. The electrical parameters extracted from the Drude model suggest a limit for Al doping efficiency.

<KWD>Keywords: ZnO; Al:ZnO; ellipsometry

<H1>1. INTRODUCTION

Zinc Oxide (ZnO) has received much attention during the last years since it is a promising material in solar cell applications requiring antireflection coatings and any other optoelectronic technology requiring transparent conducting materials for front contacts [1]. The doping of ZnO with group III elements, like Al and Ga, has emerged as a way to obtain a promising high quality transparent conductive oxide (TCO) [2]. Its high carrier concentration and wide optical band gap energy of approximately 3.3 eV has made it a suitable material for thin film solar cells [3], heterojunction solar cells [4, 5], optoelectronic devices and for the next generation of UV light emitting diodes due to the large exciton binding energy (~60meV), which allows efficient excitonic emission at room temperature [6-8]. Moreover, its nanostructures have attracted great attention as a promising functional material [9]. Focusing on the transparency and conductivity of the Al-doped ZnO (Al:ZnO) films, has turned these layers into an alternative to other TCO like ITO [10].

In spite of the enormous number of contributions dealing with the fundamental properties of doped ZnO made by scientific community, there is much fundamental research still to be done in order to fully understand the ZnO physicochemical properties modification induced by doping. In particular the analysis of the optical properties is a thematic field still open for contributions. Most of the works dealing with such issue only explore the transmittance behavior of doped ZnO films, since one of the desired characteristics of these layers is a good transparency in a wide spectrum range. However, in order to link more accurately the film electrical and optical properties, an approach based on ellipsometry which allows a more extended optical characterization would be more adequate. Variable Angle Spectroscopic Ellipsometry is a non-destructive, non-contact technique that allows determining simultaneously optical, electrical and structural properties of multilayer samples [11]. There are several works analyzing the optical response of ZnO [12] and Al:ZnO [13], modelling the dielectric function by means of Cauchy functions. Other works analyze solely the bandgap region [14], where most of the divergences among the authors are due to the presence of strong excitonic effects; however, the vast majority make an effort to describe the dielectric properties of Al:ZnO in a broader spectrum [15-17] through several models. What has been found is that there is not a unique method for describing the optical properties in the whole spectrum, and given that in most of the works the analyzed samples show just one doping level, there are not too many sources which correlate doping level and optical properties. In this work, ZnO and Al:ZnO films are deposited onto silicon wafers and quartz substrates by magnetron sputtering with the aim to analyze the behavior of