Improvement of textured AlCu with Ta underlayer on $LiNbO_3$ substrate

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Abstract

Improving the lifetime of Surface Acoustic Wave filters requires reduction of electromigration effects. We report on the growth mechanism of $AlCu_{2\%}$ film deposited by E-Beam Physical Vapor Deposition technique. State of the art shows that the introduction of an underlayer that alters the surface free energy can change a film's growth mode or improve the earliest stages of film formation. In this work, this will be achieved by using an ultra-thin (<5nm) Ta underlayer between the $LiNbO_3$ substrate and the $AlCu_{2\%}$ film. The effects of Ta underlayer on the microstructure of $AlCu_{2\%}/LiNbO_3$ films is investigated. An increase in the surface energy of the $LiNbO_3$ substrate is observed with the addition of 1.3nm thick Ta underlayer. Crystalline quality of $AlCu_{2\%}$ thin film with a Ta underlayer is measured with XRD techniques. A post-deposition heat processing is also used to recrystallize the films. The $AlCu_{2\%}/1.3Ta/LiNbO_3$ film annealed at 250°C improved the electrode quality with the increasing of 16% of grain size.

Keywords: Ultrathin underlayer, crystalline quality, grains size, $AlCu_{2\%}$, electromigration, $LiNbO_3$, SAW.

INTRODUCTION

Today, the evolution of telecommunications with 5G requires addressing new frequency bands [1]. Radio frequency modules must match these new specifications and especially the components of these modules. Until now, the filters of cell phone modules consist of bulk or surface elastic waves components [2]. To continue to use these passive components, the new specifications

require to increase their frequencies and thus to decrease their size. Size reduction combined with the required power level for 5G accelerate component degradation phenomena, such as electromigration phenomenon.

Surface Acoustic Wave (SAW) filters are usually composed of electrodes based on Aluminum (Al) material deposited on a piezoelectric substrate such as Lithium Niobate ($LiNbO_3$) or Lithium Tantalate ($LiTaO_3$) [2]. In this context, durability improvement of the electrodes is studied by many authors, like using epitaxy [3], alloys [4] or stacking [5] electrodes to prevent electromigration. Our study focuses on a simple and a cheaper approach than those cited above. The solution has to be compatible with $AlCu_{2\%}$ electrodes obtained by the lift off and very currently used for SAW filter metallization.

We start by an overview of solutions to decrease the electromigration phenomenon in SAW devices. Based on the state of the art, we choose to study the effect of Ta underlayer to limit the electromigration mechanism. The grain size (GS) of $AlCu_{2\%}$ is measured on (YX*l*)/128° $LiNbO_3$ substrates to determine the optimum Ta thickness. This measurement is achieved by means of XRD characterization and Scherrer equation on as-deposited samples and after the application of a heat processing dedicated to metal crystallization.

STATE OF THE ART

The electromigration (EM) phenomenon consists in an atomic displacement due to a momentum transfer to metal atoms which is significantly affected by temperature and stress [6]. Three main mechanisms exist: bulk, surface and grain boundary diffusion. The preponderant mechanism depends on the material considered. The grain boundaries (GB) diffusion is ruled by atoms transport mechanism for EM in the Al films. A stronger texture (meaning large grain) allows

obtaining less of large-angle GB and greater coincidence-site lattice (CSL) boundaries [7], [8]. These kinds of boundaries have a low inter-granular atomic-diffusion rate [7], [8]. Moreover, larger grains exhibit lower surface-to-volume ratios, which means less grain boundaries [9], what reduces pathways of Al atoms migration. High-quality crystalline Al film is a strategy to improve electrode resistance to EM.

Our $AlCu_{2\%}$ films are prepared at room temperature by electron beam evaporation. For Al films, an annealing processing following the deposition, from 250°C to 350°C in vacuum for 3 hours, has been considered to reduce strain generated during fabrication and to increase the crystallinity [10]. According to the phase diagram of A1-Cu alloys, the presence of 2% of Cu modifies the recrystallization temperature for the AlCu alloy films.

Moreover, the structure quality of AlCu films produced by electron beam evaporation may be improved by the addition of a thin underlayer between substrate and electrode film. This is due to the surface energy between all layers. The underlayer can be based on Ti, Cr, Zr, Co, Ni, Cu and Y [11]–[14]. Ti underlayer is mainly used due to its compatibility with standard processes in microelectronics. However, Colgan *et al.* reported that the Ti - Al interface is not stable at 350°C, due to the formation of Al_3Ti phase [15]. Nüssl *et al*. demonstrated that an ultra-thin Ti underlayer on a highly oxygen saturated surface like $LiTaO_3$ and $LiNbO_3$ is oxidized into TiO_2 during Al deposition at 200°C [16]. Nevertheless, Vogel *et al*. has found that Ti-based interfaces on $LiNbO_3$ and $LiTaO_3$ were stable up to 300 °C [17]. Another underlayer seems to be interesting to investigate. Colgan *et al*. showed a higher stability of Ta-Al interface, with a $TaAl_3$ phase occurring at 525°C and Vogel *et al*. attested that the Ta interface on $LiNbO_3$ was stable up to 600°C. Ti may

not be stable from 300°C, unlike Ta which can withstand these conditions [17]. Therefore, in this work, we consider using Ta as an intermediate layer since it can withstand these temperatures.

In our previous work [18], we have investigated the influence of Ta thickness underlayer on the free surface energy of a $LiNbO_3$ substrate. The 1.3nm Ta underlayer was found to be the best candidate [18]. We have demonstrated that 1.3nm of Ta increases the surface free energy of $LiNbO_3$ substrates. The objective of this study is to demonstrate that 1.3nm-thick Ta underlayer increases the GS of $AlCu_{2\%}$ films.

CRYSTAL QUALITY OF AlCu2% WITH Ta UNDERLAYER

In order to investigate the effect of the Ta underlayer on the microstructure of the $AlCu_{2\%}$, $AlCu_{2\%}$ 100nm-thick film is deposited onto several thicknesses of Ta (0, 1.3, 5 and 20nm) on congruent 100mm 128°-rotated Y-Cut $LiNbO_3$ wafers, by electron beam evaporation in a Balzers BAK760. Deposition of Ta underlayers was carried out with a rate of $0.3nm.s^{-1}$ at room temperature, after the chamber was pumped down to 10^{-6}mbar using a vacuum system consisting of a primary pump and a cryopump. Finally, without breaking vacuum, AlCu2% films were evaporated at a rate of $1nm.s^{-1}$. Its thicknesses is monitored as well as seed layer ones using an in-situ quartz crystal microbalance. Following this deposition, a crystallization step is achieved at 250°C and 350°C for 3 hours in vacuum to determine the appropriate temperature. Finally, the GS is calculated using XRD analysis on every sample using the Scherrer's equation [19].

The structural characterization of the AlCu2% film is performed by XRD. FIG. 1 shows XRD diffractograms for the AlCu2% film deposited on $LiNbO_3$ substrate (red curve) and for a bare $LiNbO_3$ substrate (black curve). The characteristics of the Al peak (intensity and Full Width at Half Maximum – FWHM) can be used to determine the GS in $AlCu_{2\%}$ films. FIG. 1-b shows

diffractograms of the $AlCu_{2\%}$ film measured in θ–2θ mode where diffracted signals from the substrate do not allow to observe the diffraction peaks related to the 100nm thick $AlCu_{2\%}$ film. FIG. 1-a shows diffractogram of the AlCu2% film obtained by grazing incidence XRD mode with a grazing incidence angle of 0.80°. Lim et *al*. demonstrated that the use of a small angle of incidence allows the X-ray to better probe the lattice of the thin film and consequently increases diffracted signals due to the film [20]. Consequently, during our experiments, both modes, (grazing and θ-2θ) are mandatory.

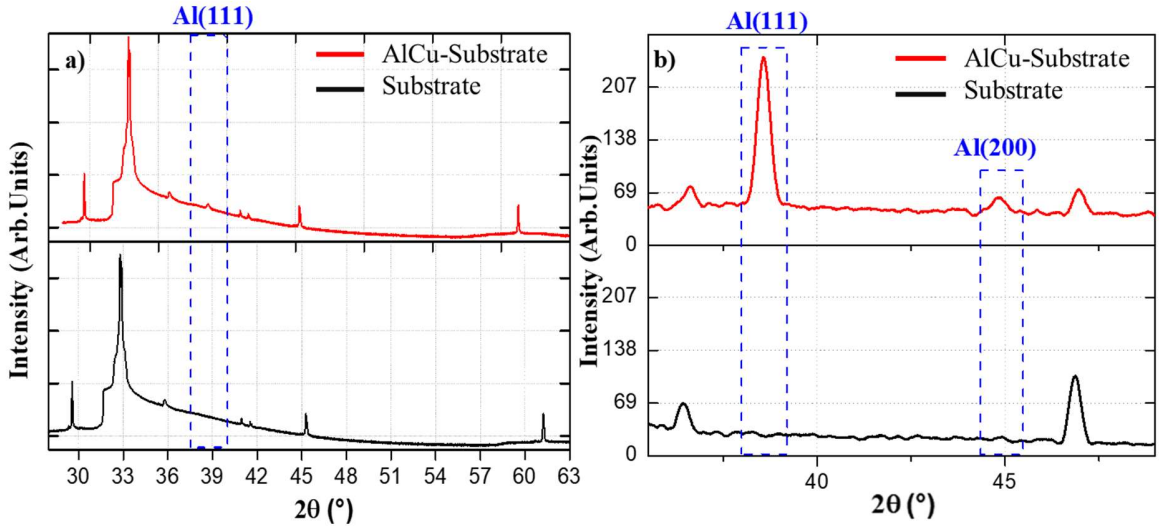

FIG. 1: X-ray diffractograms for an AlCu film (100 nm) deposited on $LiNbO_3$ (red curve) and for a raw $LiNbO_3$ substrate (black curve), obtained by grazing mode (GIXRD) left figure (a) and θ-2θ mode right figure (b)

The grazing mode enables to increase diffracted signals due to the film compared to those of the substrates. This allows one to identify a diffraction peak detected at $2\theta = 38.56°$. This peak is present in the diffractogram of the AlCu2%-$LiNbO_3$ stack (red curve in FIG. 1) and is missing in the diffractogram of the raw substrate (black curve in FIG. 1). With this mode only the AlCu film is probed. This allows to get rid of the influence of the substrate. According to International Centre

for Diffraction Data (ICDD) pdf #00-001-1176, two peaks are indexed as the (111) plane at $2\theta =$ 38.56° and (200) at $2\theta = 44.83°$ for Al. Intensity ratio reveals that the crystallites in the $AlCu_{2\%}$ film are orientated in following the [111] direction preferentially. This means that the AlCu film deposited on $LiNbO_3$ in initial form has (111) texturing. The FWHM of this peak is calculated using Scherrer's equation to estimate the GS of AlCu films. It allows to derive the GS of the AlCu film from the integral width of the (111) diffraction peak.

The equation (1) proposed by Scherrer [19] relates the width of a diffraction peak to the average dimension of crystallites in a polycrystalline material as:

$$\beta_s(2\theta)_{hkl} = \frac{K\lambda}{D\,Cos_{\ hkl}} \qquad (1)$$

where D is the average GS of the polycrystalline in a direction normal to the diffracting plane hkl (nm), λ is the X-ray wavelength (CuK_α λ=1.5418Å), θ is the Bragg reflection angle (rad), K is a Scherrer constant (K=1) and β_s is the crystallite size contribution to the peak width (integral or FWHM) (rad). Our data are collected in the Bragg-Brentano configuration at ambient conditions with a scintillation detector from 2θ = 27.9° to 91.9° with a 2θ step size of 0.0027° and using the above-mentioned CuK_α wavelength.

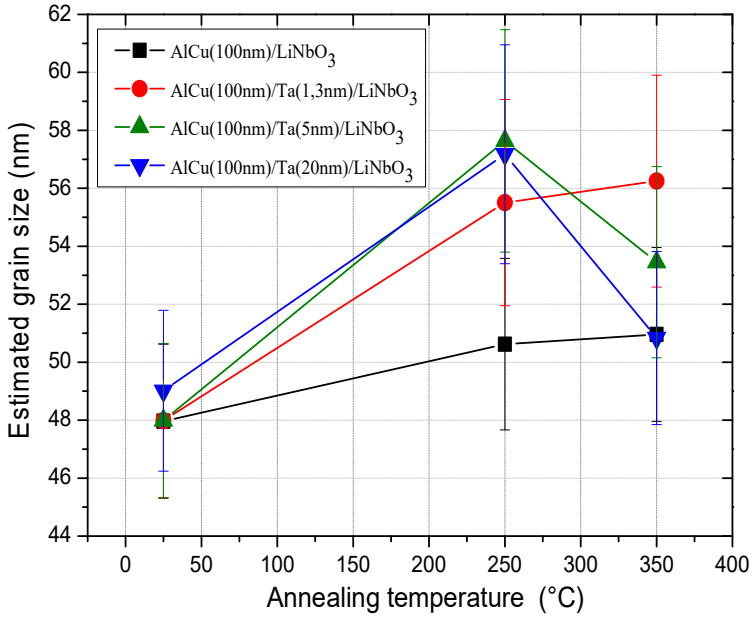

FIG. 2: Evolution of the GS as a function of Ta underlayer thicknesses and temperature of the heat treatment. Thickness of AlCu2% is 100nm, and Ta underlayer thicknesses are 0, 1.3, 5 and 20nm.

The GS *vs* annealing temperature and as a function of Ta underlayer thickness is shown in Fig. 2. The GS values vary between 48.0nm ± 2.7nm and 51.0nm ± 2.8nm for as-deposited AlCu-$LiNbO_3$ samples (black curve). After deposition, no significant improvement is observed. A post-deposition heat processing is performed to recrystallize the films. After that, most samples presented larger GS. This improvement is more significant with Ta underlayers. Therefore, the recrystallization step is mandatory to increase the GS.

As shown in Fig. 2 at 250°C the grain size increases for all samples with Ta underlayer, whereas at 350°C, only Ta 1.3nm-thick configuration keeps on increasing. As a result, the optimal condition for improving GS is the use of 1.3nm-thick underlayer and a heat processing at 250°C.

CONCLUSION

$AlCu_{2\%}$ electrodes on (YX*l*)/128° $LiNbO_3$ substrates are typically used for SAW filters. High-quality $AlCu_{2\%}$ poly-crystalline film reduces the electromigration phenomenon that occurs when SAW filters are stressed. In this way, the addition of a thin Ta underlayer has been studied. The observed influence of the proposed approach on as-deposited samples is not spectacular but the resulting electrodes exhibit a higher GS when they are thermally processed at 250°C and 350°C in vacuum for 3 hours. The sample with ultra thin 1.3nm Ta underlayer allows to achieve stable temperature behaviour with crystallites reaching a diameter of 56 nm at 350°C. Therefore, such a multi-layer film is considered as a relevant candidate to improve lifetime of SAW components.

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