Proc. 2009 IEEE International Ultrasonics Symposium, Rome, Italy, Sept. 20-23, 2009, pp. 2635-2638

Transformation of Surface Acoustic Waves into Boundary Waves in Piezoelectric/Metal/Dielectric Structures

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***Abstract* — A universal technique was developed for analysis of SAW and boundary waves (BW) in Piezoelectric/Metal/ Dielectric structures with uniform metal film sandwiched between piezoelectric substrate and dielectric overlay, and dielectric overlay thickness varying between zero and infinite value. This technique was applied to 128°YX LN with Cu and silica glass films. For each mode propagating in this structure, continuous transformation of the wave polarization and distribution of its energy along the vertical axis were analyzed as functions of metal and dielectric film thickness. The found dependences reveal the mechanisms of wave transformation from SAW to BW.**

Keywords - SAW, boundary wave, multilayered structures, dielectric film, 128°YX LN

I. INTRODUCTION

Boundary waves (BW) propagate along the interface between two half-infinite media [1, 2]. Recently, this type of waves attracted attention of SAW designers as alternative to common SAW or leaky SAW (LSAW) propagating in piezoelectric substrate with periodic grating and thin dielectric overlay (e.g. material with opposite sign of TCF, to improve temperature characteristics). Application of BW, instead of SAW, helps to avoid problems of packaging and decrease sensitivity of device characteristics to the quality of crystal surface. The most promising combination of materials is LN substrate with silica glass (SiO_2) upper and copper electrodes between them [1]. This combination provides simultaneously high electromechanical coupling, improved temperature behavior and low propagation losses (due to localization of BW in heavy metal film).

In SAW devices utilizing boundary waves, the thickness of dielectric overlay usually does not exceed one-two wavelengths. Analysis of the boundary wave structure and, in particular, clarifying the mechanism of transformation of SAW into BW with increasing thickness of dielectric overlay, can be very helpful in estimation of proper thickness of dielectric film and more accurate simulation of device characteristics for different types of boundary waves.

II. METHOD OF ANALYSIS

In SAW devices, IDTs or periodic metal arrays are used for generation, transformation and detection of SAW. However, the mechanism of wave transformation from SAW into BW with increasing thickness of dielectric overlay is mostly determined by the properties of a substrate. Hence, this mechanism can be understood from more simple simulation of wave behavior in a uniform metal film sandwiched between piezoelectric substrate and dielectric overlay.

Matrix method [3] provides a universal technique for analysis of multilayered structures. After multiplication of transfer matrices of *n* layers in upper half-space and *m* layers in lower half-space, the solution at the interface between these two half-spaces is found from impedance boundary equation, with OC or SC electrical condition at metallized interface. A special case of unloaded substrate or a substrate covered with thin metal and dielectric films can be simulated if most upper dielectric half-space is characterized by very low values of elastic constants and mass density (air). This approach assumes arbitrary number of finite-thickness films in both half-spaces.

An important requirement to a method of analysis is a possibility of varying film thicknesses in a wide range, including few or few hundred wavelengths (λ). Since transfer matrix multiplication evokes numerical noise when $h>5\lambda$, analysis of *transmitted* and *reflected* partial modes is performed separately, for each layer, to calculate transmission and reflection matrix coefficients [4]. With this modification, the developed universal technique enables analysis of SAW and LSAW in a substrate, in a substrate with metal film of variable thickness, and with deposition of dielectric film over the metal, when the thickness of film grows from zero to infinite value. Such analysis reveals the mechanisms of wave transformation from SAW into BW and helps to estimate effective thicknesses of metal and dielectric required to obtain the desired wave characteristics.

III. RESULTS OF CALCULATIONS AND DISCUSSION

The universal technique described above was applied to 128°YX LN with Cu film and dielectric SiO_2 overlay. The calculated velocities of SAW and LSAW modes are shown in Fig.1, as functions of metal and dielectric film thicknesses.

Orientation 128°YX is characterized by special properties, compared to other rotated YX-cuts of LN, because slow shear limiting bulk wave (BAW2 in Fig.1) is *exceptional* and satisfies stress-free boundary conditions [5,6]. As a result, when the surface is loaded by thin metal film (Fig.1a), SH-polarized quasi-bulk mode SAW2 arises from BAW2, in addition to SAW1. This mode has nearly zero piezoelectric coupling but plays an important role in transformation of SAW into BW. Leaky SAW does not exist in unloaded substrate and appears only with sufficient metal thickness. For Cu it is about 0.11λ. With further increasing metal thickness, the velocities of SAW1, SAW2 and LSAW decrease. Electromechanical coupling of SAW1 grows while other modes stay nearly uncoupled (Fig.1a).

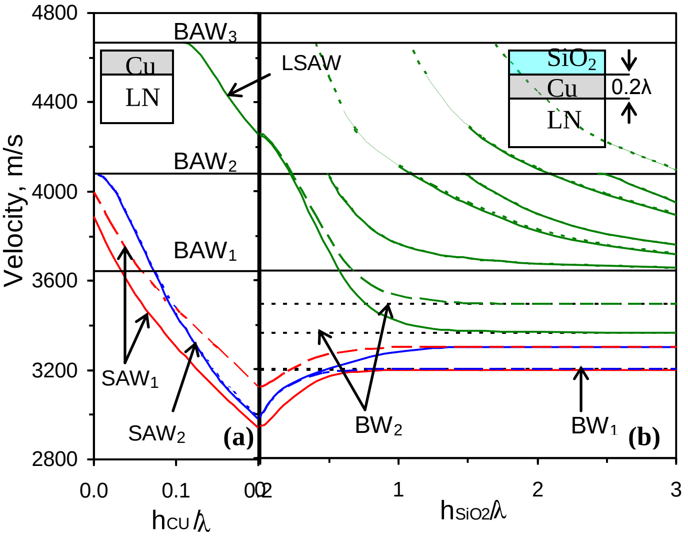

Fig.1. Calculated velocities of surface acoustic modes propagating in 128°YX LN with Cu film (a), as functions of metal film thickness, and in LN with Cu film (h/λ=0.2) and SiO_2 overlay (b), as functions of SiO_2 overlay thickness. BAW1 is the velocity of shear bulk waves in SiO_2, BAW2 and BAW3 refer to limiting bulk waves in LN.

If metal thickness is fixed (h_{Cu}=0.2λ) and SiO_2 film is deposited over this structure, the velocity of LSAW mode continues to decrease with SiO_2 thickness while the velocities of two SAW modes increase (Fig.1b). When h_{SiO2} ≈1.5λ, the modes SAW1, SAW2 and LSAW transform into boundary waves, BW1 and BW2. Higher velocity LSAW modes, which arise from BAW2 or BAW3 (fast shear limiting BAW in LN) at nonzero SiO_2 film thicknesses, do not transform into BWs because of energy leakage into SiO_2 half-space.

With increasing thickness of dielectric overlay, the properties of boundary waves become less sensitive to mechanical displacements on its top surface, but parameters of SAW devices can be affected by reflections from this surface. Therefore, in addition to velocities it can be helpful to estimate the distribution of wave energy across the multi-layered structure, at different thickness of dielectric film.

The numerical technique described in Section II enables calculation of polarization components versus depth for each SAW or LSAW mode. Fig.2 and Fig.3 demonstrates how polarizations of two SAW modes existing in a substrate change with increasing Cu film thickness from zero to 0.2λ. Fig.4 shows further transformation of the waves with increasing thickness of additional SiO_2 overlay, while h_{Cu} is fixed (0.2λ). Both types of electrical conditions are considered for metal film, OC and SC.

In a substrate without films, mode SAW1 is nearly sagitally polarized (Rayleigh-type) and mode SAW2 is SH-type quasi-bulk wave, for both electrical conditions. With increasing metal thickness, the behavior of the waves depends on electrical condition. For OC metal film (Figs.2b, 3b), maximum interaction between two modes occurs at h_{Cu}≈0.1λ, which results in maximum deviation of SAW1 from sagitally-polarized mode (U_{SH} grows). With further increasing Cu thickness to h_{Cu}=0.2λ, SAW1 and SAW2 transform, respectively, into the waves with pure sagittal and SH polarizations. For SC metal film (Figs.2a, 3a), the velocities of two SAW modes approach each other with increasing Cu thickness. Due to interaction between them, both modes have mixed type of polarization at h_{Cu}=0.2λ.

Transformation of two SAW modes continues when SiO_2 overlay is deposited over Cu film, h_{Cu}=0.2λ (Fig.4). After strong interaction between two modes at h_{SiO2}≈0.5λ, SAW1-SC (Fig.4a) and SAW2-OC (Fig.4d) transform into SH-type boundary wave BW1 with electromechanical coupling about 0.3%. At the same time, SAW1-OC (Fig.4b) converges with SAW2-SC (Fig.4c) and maximum amplitude of both modes moves fast from interface to the top surface of SiO_2, with increasing film thickness. Hence, this couple of modes does not transform into BW.

The depth profile of BW1, which appears due to interaction between SAW1 and SAW2, is shown in Fig.4e and looks similar for OC and SC conditions, with nearly zero U_L and U_{SV} components. Small difference in the wave structure agrees with low piezoelectric coupling of BW1.

It should be mentioned that even for SAW modes, which finally transform into BW, part of wave energy moves with increasing SiO_2 thickness from the interface to the top surface of SiO_2. For h_{SiO2}=(1-2)λ, the wave is mostly confined in Cu film and around it, but for h_{SiO2}>(3-3.5)λ its amplitude grows fast near the top surface of SiO_2 (Fig.3). Besides, polarization at the top surface is different for OC and SC electrical conditions in Cu film. This can be a reason of strong reflections from the top surface of SiO_2 overlay when its thickness is about few wavelengths.

The behavior of LSAW is more complicated. This mode arises from the fast shear BAW in LN (BAW3 in Fig.1). Fig.5 shows LSAW velocity and attenuation coefficient as functions of Cu film thickness. Attenuation tends to zero when LSAW degenerates into BAW3. The existence of low-attenuated quasi-bulk wave is explained in Fig.6a, which shows slownesses of three bulk waves in the sagittal plane. Around X-axis there is a symmetric concavity of the fast shear BAW branch, which means simultaneous propagation of two bulk waves along the surface, with $V=V_{fast\ shear\ BAW}$. The Pointing vectors of BAWF1 and BAWF2, i.e. $\mathbf{P}_1$ and $\mathbf{P}_2$, are parallel to the surface, while the wave vectors are tilted symmetrically into the upper and lower half-space. A combination of BAWF1 and BAWF2 gives *composite limiting BAW* [7]. Polarization vectors of two bulk waves ($\mathbf{U}_1$ and $\mathbf{U}_2$) are also tilted symmetrically with respect to X-axis. Their combination $\mathbf{U}_{CBAW}=\mathbf{U}_1+\mathbf{U}_2$ is parallel to X axis and thus can satisfy stress-free mechanical boundary conditions. In this case, CBAW becomes LH-polarized *composite exceptional wave* [8].

The calculated polarization versus depth dependences are shown for LSAW mode when h_{Cu}=0.11λ (Fig.6b) and h_{Cu}=0.2λ (Fig.6c). In the first case, $V \approx V_{fast\ shear\ BAW}$ and the wave is quasi-longitudinal at LN/Cu interface, as expected. In the depth of LN, all components of polarization are present and show oscillations with nearly constant amplitude, which proves the quasi-bulk nature of LSAW. With increasing Cu thickness, LSAW better localizes near the surface and its polarization stays nearly longitudinal at LN/Cu interface. At h_{Cu}=0.2λ, LSAW attenuation increases and U_{SH} component does not attenuate in the depth of LN.

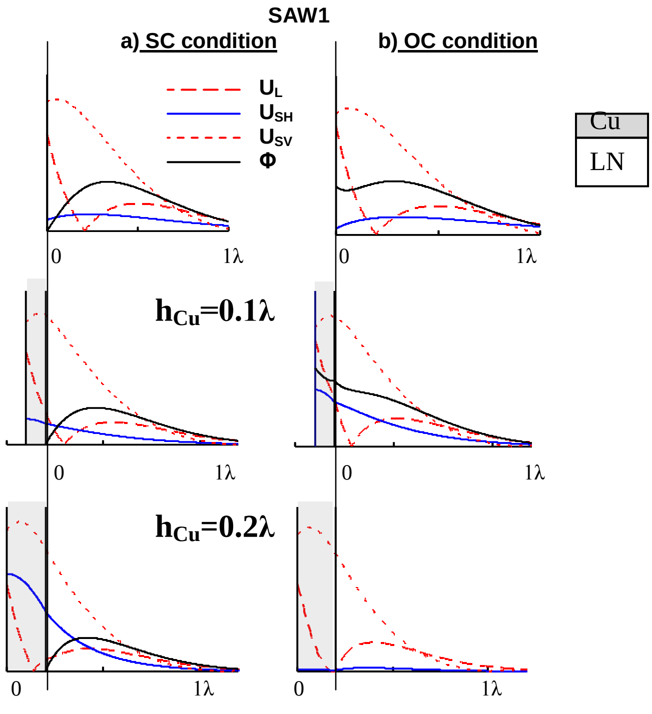

Fig. 2. Transformation of wave polarization versus depth with increasing metal film thickness, in 128°YX LN with SC (a) and OC(b) Cu film, **mode SAW1**

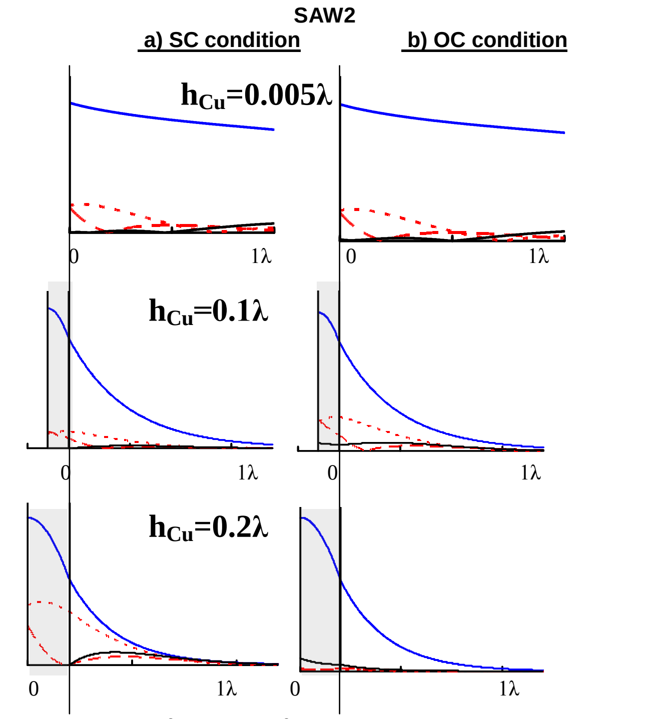

Fig. 3. Transformation of wave polarization versus depth with increasing metal film thickness, in 128°YX LN with SC (a) and OC(b) Cu film, **mode SAW2**

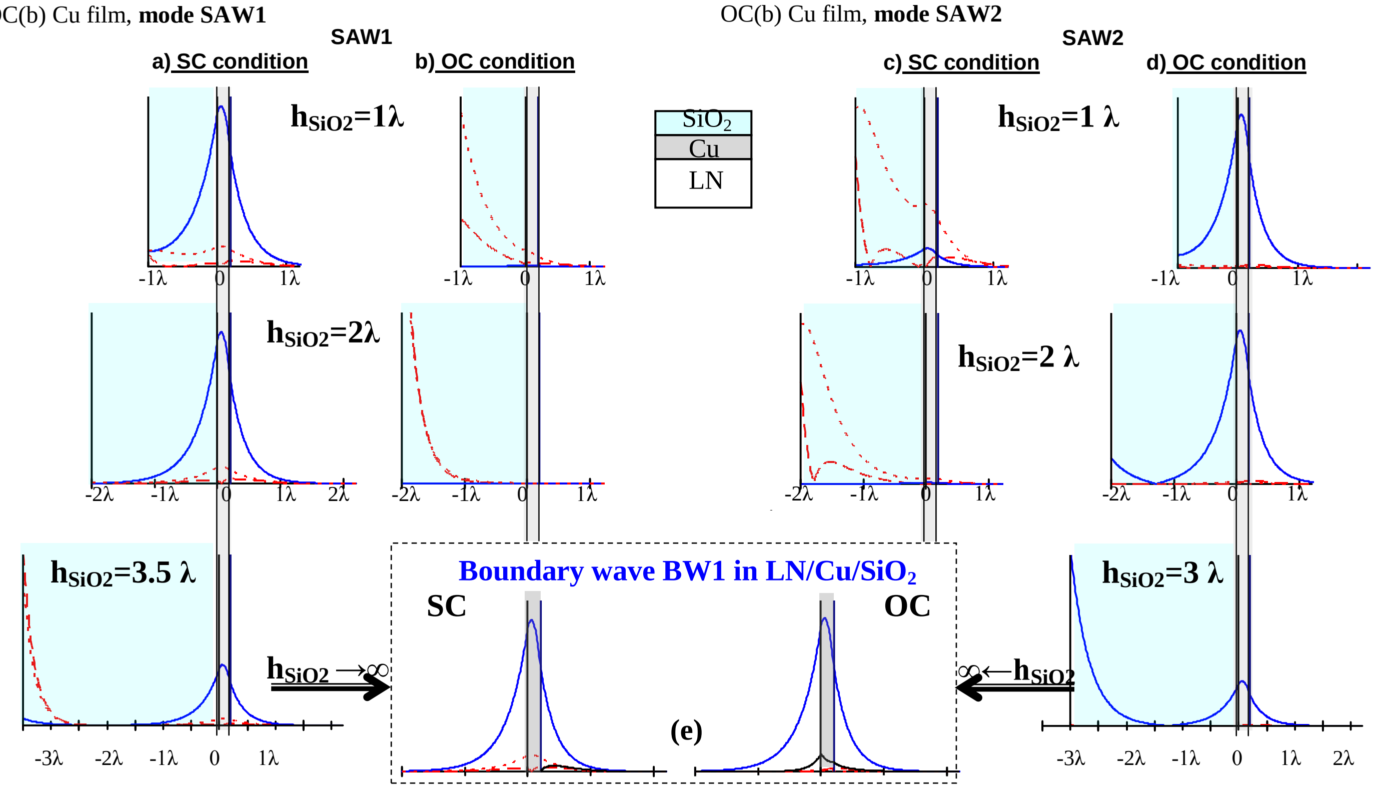

Fig. 4. Further transformation of **SAW1** (a, b) and **SAW2** (c, d) into Boundary Wave **BW1** (e) with increasing thickness of SiO_2 overlay on top of 128°YX LN with **SC**(a, c) and **OC** (b, d) Cu film (h/λ=0.2).

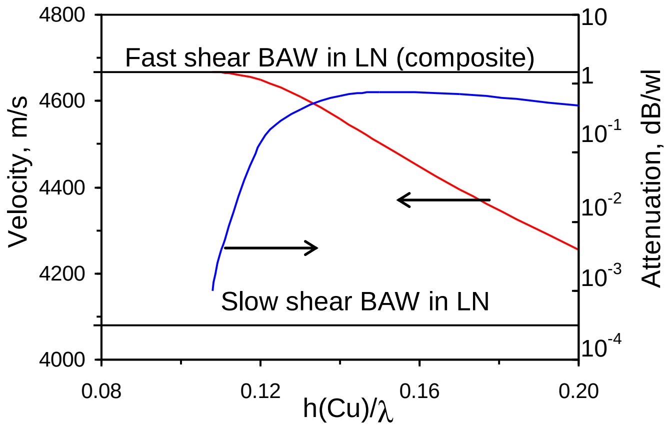

Fig. 5. LSAW velocity and attenuation as functions of Cu film thickness, in 128° LN with Cu overlay (SC condition)

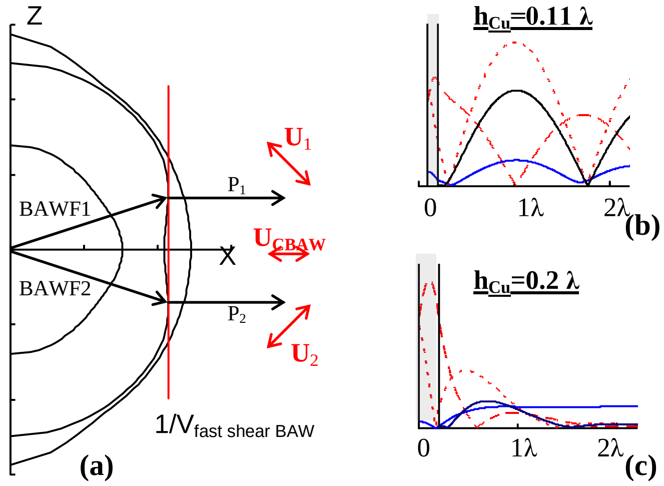

Fig. 6. Slownesses of bulk waves in the sagittal plane of 128°YX LN, which explain the structure of *composite* fast shear *limiting BAW* (a). Polarization of wave is shown in 128°YX LN with Cu film, when LSAW arises from CBAW, h_{Cu}=0.11 λ (b) and at h_{Cu}=0.2 λ (c),.

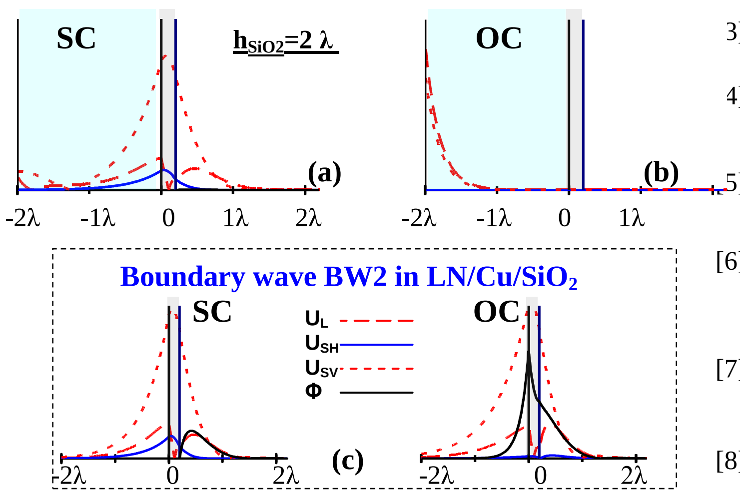

Fig. 7. Polarization of **LSAW mode** in 128°LN/Cu/SiO$_2$, h_{Cu}=0.2λ, h_{Sio2}=2λ (b). Polarization of boundary wave **BW2** (c)

LSAW transforms into SAW with deposition of SiO$_2$ overlay, when h_{SiO2}>0.25λ and further transforms into boundary wave BW2, as shown in Fig.7a. This wave has higher electromechanical coupling k^2 than BW1, about 7.6%, which agrees with the calculated structure of BW2 (Fig.7c). The amplitude increases at the top surface of SiO$_2$ overlay, when h_{SiO2}>0.5λ for SC condition and h_{SiO2}>3λ for OC condition.

IV. Summary

A universal technique was developed for analysis of SAW and boundary waves in Piezoelectric/Metal/Dielectric structures and applied to 128°YX LN with Cu film and silica glass overlay. For each mode propagating in this structure, continuous transformation of wave polarization and distribution of its amplitudes along the depth were analyzed with increasing metal and dielectric film thicknesses. The found dependences reveal mechanisms of wave transformation from SAW into BW. With increasing thickness of SiO$_2$ overlay, three surface modes existing in 128°YX LN covered by thin Cu film interact and eventually build two boundary waves, one of which is SH-type and the second is nearly polarized in the sagittal plane. The mechanism of wave transformation is expected to change insignificantly if uniform metal film is replaced by periodic grating, though typical thicknesses will change.

The observed behavior of surface modes in 128°YX LN and the details of its transformation into boundary waves should be generalized with caution to arbitrary rotated YX-cut of LN, because the analyzed orientation has some specific properties.

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