Ultrasonics 56 (2015) 318–324

Contents lists available at ScienceDirect

Ultrasonics

journal homepage: www.elsevier.com/locate/ultras

Surface acoustic wave reflection/transmission at vertical borders of piezoelectric substrates

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ARTICLE INFO

Article history:
Received 19 June 2014
Received in revised form 27 July 2014
Accepted 12 August 2014
Available online 27 August 2014

Keywords:
Surface acoustic waves
Scattering
Reflection
Transmission
Finite element method

ABSTRACT

The paper studies by the finite element method the harmonic surface acoustic wave scattering at 90° corners of piezoelectric substrates. The SAW is incident perpendicular to the vertical border. The dependencies of the reflection and transmission coefficient on the radius of the fillet at the corner are found for 128°YX and YZ $LiNbO_3$ as well as ST-X SiO_2 substrates. In particular, the obtained results reveal that, like in the case of isotropic solids, the magnitude of the reflection coefficient first increases with the fillet radius to wavelength ratio r/λ, reaches a maximum at $r/\lambda \approx 0.3 - 0.5$, and then decreases tending to zero. The magnitude of the transmission coefficient across the rounded corner first decreases, reaches a minimum at $r/\lambda \approx 0.3 - 0.5$, and then increases up to a value around which it slightly oscillates as r/λ increases. It is demonstrated that if the substrate is anisotropic, then in the general case a SAW is scattered off differently at the right-hand border and the left-hand border. The difference between the "right-hand" and "left-hand" transformation coefficients can be very substantial. Computations for YZ $LiNbO_3$ illustrate possible levels of the anisotropy of the scattering for mutually reverse directions of incidence. It is shown that if the substrate is specially oriented, then the scattering from the right-hand border is identical to the scattering from the left-hand border. There are four types of such orientations. Examples of the specially oriented substrates are 128°YX $LiNbO_3$ and ST-X SiO_2.

1. Introduction

Piezoelectric materials are widely used as substrates for the manufacture of surface acoustic wave (SAW) devices [1,2]. It is natural that an actual substrate is of finite size, so the SAW generated by an interdigital transducer (IDT) on one of the substrate faces almost always propagates as far as substrates edges. When meeting a border, the SAW is partially reflected off, changing the direction of propagation on the working face, partially transmits on the neighboring face, and partially transforms into bulk waves irradiated from the junction of borders towards the interior of the substrate. In view of anisotropy the transmitted and the reflected SAWs can be strongly different by their structures from the incident SAW.

The scattering problem for SAW at the substrate edge is of interest from the viewpoint of practical applications. In particular, it is helpful to know the amplitude of the reflected SAW in order to be able to estimate the electric signal induced by this wave. It is also of interest to know to what extent one can vary the reflection and the transmission by changing the shape of the face junction. The transmission of the SAW from one face to another can be utilized for the generation of SAW on the face where for some reasons the IDT cannot be created.

The analysis of the scattering phenomenon is of scientific interest as well, broadening one's understanding of basic specific features of the SAW propagation in anisotropic media. For instance, one should think that the reflection coefficients of the SAW incident normally on the left-hand side and the right-hand side borders of the substrate are different because of the anisotropy. It is of interest to know how significant this difference can be in typical situations. A similar effect takes place when a SAW is scattered from a surface irregularity in anisotropic substrates. The reflection coefficients from a symmetric irregularity are different for the SAW incident from the right and the left [3]. In contrast, the transmission coefficients are always identical for both the direction of incidence due to the reciprocity theorem. When the SAW is scattered by the substrate edge the equality of the transmission coefficients does not hold, but in this case the reciprocity theorem also plays a role to be discussed in what follows.

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http://dx.doi.org/10.1016/j.ultras.2014.08.012
0041-624X/

The scattering of SAW at the edge of piezoelectrics, or, speaking more generally, in piezoelectric wedges, has been studied analytically by an approximate method only as applied to the Bleustein–Gulyaev wave in materials of hexagonal symmetry and the wedge faces were metallized [4,5]. The method used in [4,5] was a generalization of the method put forward in Refs. [6,7] as applied to isotropic solids. The approximation consisted in that the contribution of bulk waves was not taken into account exactly. Note that various approximate methods were also suggested to investigate analytically the SAW scattering in isotropic wedge-like domains (see, e.g., [8], ch. 12).

To the best of our knowledge, there is no papers where the SAW scattering at the border of piezoelectric substrates is studied exactly analytically or numerically. On the other hand, a number of works has been published where the Rayleigh wave scattering problem in isotropic substrate is solved exactly. In a part of the papers the boundary-value problem is first reduced with help of fairly involved evaluations to integral equations that are eventually solved numerically [9–18]. In the other papers the wave equations are directly solved by a numerical method: finite difference method [19], boundary element method [20], mixed finite element/finite difference method in time domain [21]. It is worth noting that these methods yield practically identical values for the reflection and the transmission coefficients.

In our previous work [22] we investigated by FEM the Rayleigh wave scattering by vertical edges in isotropic materials. The computations were performed in frequency domain, i.e., the scattering of a plane harmonic SAW was studied rather then the scattering of a pulse as it had been done in Ref. [21]. The so-called perfectly matched layer (PML) [23–27] was implemented in order to spatially truncate the computational domain. Note that in order to validate our method we have reproduced in [22] results[1] obtained in Refs. [9–21].

In this work we apply FEM in combination with PML method to simulate the scattering of the SAW of general polarization in 128°YX $LiNbO_3$ and ST-X SiO_2 and of the sagitally polarized SAW in YZ $LiNbO_3$. These cuts are often used for the production of acoustoelectronic devices [1,2].

2. Statement of the problem

Let a piezoelectric substrate occupy the quarter-space $z, x < 0$. The remaining three quarters are the vacuum. The incident harmonic SAW propagates with frequency ω and velocity v_I along the axis x from $x = -\infty$ towards the vertical edge $x = 0$. The mechanical displacement $\mathbf{u}_I(\mathbf{r}, t)$ and the electric potential $\varphi_I(\mathbf{r}, t)$ created by this wave in the substrate are $\mathbf{U}_I(\mathbf{r}, t) = \mathbf{U}_{0I}(z)\exp[i(k_I x - \omega t)]$, where $\mathbf{U}_I(\mathbf{r}, t) = (\mathbf{u}_I, \varphi_I)^T$ stands for the four-component vector-column, $\mathbf{U}_{0I}(z)$ is defined analogously and describes the z-dependence of the wave field, $k_I = \omega/v_I$.

When striking the edge (plane) $x = 0$ the incident SAW gives rise to the scattered fields $\mathbf{u}_{SC}(\mathbf{r}, t)$ and $\varphi_{SC}(\mathbf{r}, t)$. These fields are found by solving the boundary-value problem by FEM using a program written on the basis of COMSOL Multiphysics and MATLAB.

Eventually we want to determine the amplitudes of the reflected SAW $\mathbf{U}_R(\mathbf{r}, t) = \mathbf{U}_{0R}(z)\exp[-i(k_I x + \omega t)]$ and of the transmitted SAW $\mathbf{U}_T(\mathbf{r}, t) = \mathbf{U}_{0T}(x)\exp[-i(k_T z + \omega t)]$, where $k_T = \omega/v_T$ and v_T is the velocity of the SAW on the plane $x = 0$. These amplitudes are calculated, like in our earlier papers [28–33], with the help of the spacial Fourier transform by extracting the harmonic $k_x = -k_I$ of the displacement $u_{SC,z}(\mathbf{r}, t)$ at $z = 0$ and the harmonic $k_z = -k_T$ of the displacement $u_{SC,x}(\mathbf{r}, t)$ at $x = 0$, respectively. The reflection and the transmission coefficients are defined as the ratio of the normal component of the mechanical displacement of the corresponding wave to the normal component of the mechanical displacement of the incident SAW.

The computational domain is depicted schematically in Fig. 1. The electric potential in the vacuum is described by the function $\varphi_V(\mathbf{r}, t)$ and obeys the equation $\Delta\varphi_V = 0$. The total mechanical displacement and the electric potential in the substrate are written in the form $\mathbf{u}_{SC}(\mathbf{r}, t) + \mathbf{u}_I(\mathbf{r}, t)$ and $\varphi_{SC}(\mathbf{r}, t) + \varphi_I(\mathbf{r}, t)$, respectively. They obey the equations

$$\nabla(\hat{\sigma}_{SC} + \hat{\sigma}_I) = -\rho\omega^2(\mathbf{u}_{SC} + \mathbf{u}_I), \ \ \nabla(\mathbf{d}_{SC} + \mathbf{d}_I) = 0, \tag{1}$$

where $\hat{\sigma}_{SC}$ and $\hat{\sigma}_I$ are the mechanical stresses produced by the scattered acoustic field and the incident SAW, respectively, $\mathbf{d}_{SC}$ and $\mathbf{d}_I$ are the electric displacements produced by the scattered acoustic field and the incident SAW, respectively, ρ is the density of the substrate. The condition $\varphi_{SC}(\mathbf{r}, t) + \varphi_I(\mathbf{r}, t) = \varphi_V(\mathbf{r}, t)$ is put on the substrate – vacuum boundary. The vanishing of the traction and the continuity of the normal component of the electric displacement on this interface are the natural boundary conditions. The conditions on the exterior boundary of the computational domain does not play any role, since the parameters of PML are chosen such that the results are to be quasi independent[2] on these conditions as well as on the size of domains 11 and 12 representing the substrate and the vacuum, respectively.

3. Results

Before discussing the results we introduce additional notation. Let us imagine that the cross-section of the substrate by the plane xz is a rectangular (Fig. 2a). Its sizes are assumed to be so big that a SAW propagates along edges AB, BC, etc. as if the substrate were half-infinite. Besides, the scattering at a corner is not affected by the other corners, i.e., the substrate around each of the four corners can be treated as a quarter-space.

The geometry of the scattering, i.e., the orientation of the surface on which the incident SAW propagates and the direction of propagation of this SAW, will be formally specified by three Euler angles (φ, θ, ψ) [1,2]. In parallel, to distinguish between different options more visually, we refer as S_{AB} to the scattering at corner B of the SAW propagating along edge AB from A to B, as S_{BA} to the scattering at corner A of the SAW propagating along edge AB from B to A, etc.

In this notation four cases will be of our interest: S_{AB}, S_{BA}, S_{CB}, and S_{DA} (see Fig. 2b–e). The reflection and the transmission coefficients are denoted by letters R and T, respectively, with subscripts indicating at the scattering option. For instance, the symbols R_{AB} and T_{AB} stand for the transformation coefficients in case S_{AB}, where the reflected SAW propagates along edge AB from B to A and the transmitted SAW propagates along edge BC from B to C. Analogous principle of ascribing subscripts will be used to identify the relative energy flow $E = |R|^2 + |T|^2 P_{tr}/P_{in}$ of the reflected and transmitted SAWs, where P_{in} and P_{tr} are the energy flows carried by the incident (reflected) and transmitted SAWs with unit amplitude of mechanical displacement on the surface,[3] respectively, e.g., E_{AB} is the total flow in the case of scattering S_{AB}.

In what follows we present the results of our computations for 128°YX and YZ cuts of $LiNbO_3$ and ST-X SiO_2.

[1] The transformation coefficients found in Ref. [12] are complex conjugate to the coefficients computed in our paper [22] as well as in Refs. [9–11]. However, this discrepancy has a simple explanation, see [22].

[2] A number of causes why in practice PML does not eliminate completely parasitic fields are discussed in Ref. [15].

[3] Notice that $|T|$ can be greater than 1 when $P_{tr} < P_{in}$.