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FEM modeling of AlN/diamond surface acoustic waves device

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Abstract

This paper describes a general finite element method (FEM) for the AC steady state analysis of two-dimensional piezoelectric devices. The method is applied to a diamond based surface acoustic wave (SAW) layered structure. We determined the penetration depth of the elastic waves corresponding to a AlN layer of 5.2 µm thick and a spatial periodicity of 12 µm. The structure admittance response shows peaks corresponding to the modes 0, 1, 2 and 3. The penetration depth in diamond is around 24 µm.

Keywords: FEM; SAW; AIN; Diamond

1. Introduction

Surface acoustic wave (SAW) filters are widely used in the frequency range from 30 MHz up to 3 GHz owing to their highly selective band-pass filtering quality and to their lower cost of production. Diamond with its highest SAW phase velocity relative to other known materials appears as a potential device-composing layer in such SAW devices [1,2]. The phase velocity v● of a SAW in such a structure depends on the tensor data of the substrate, the piezoelectric and electrode materials as well as on the geometrical shape of the electrode. It is determined by the centre frequency (f0) of the SAW filters and the spatial period (λ) of the IDTs: v● = f0 * λ. However, as the SAW is excited in the diamond layer by electromechanical conversion, a piezoelectric layer such as ZnO or AlN is required and metallic inter-digital transducers (IDTs) are therefore deposited on top of the diamond surface.

The broad variety of materials, crystallographic cuts and parameters make systematic measurements of those parameters extremely time consuming [3]. Accurate SAW filter simulations have now become indispensable for designing high quality and low-loss SAW devices [4]. Analytical and numerical studies [1,4–6] have been conducted in order to obtain an exact quantitative description of SAW devices based on a diamond surface. For such SAW devices, the finite element analysis of infinite gratings of IDTs in surface acoustic waves (SAW) is a performing tool. Thanks to the easy way of analysing complicated geometries particularly the Finite Element Method has proved to be a well suited numerical method to derive the influence of geometrical variations of the electrode's shape. The computation of one half period of the infinite structure with the application of inverted periodical boundary conditions allows us the analysis of the total device geometry [7]. However, FEM suffers from immense computational expense, which is necessary if extremely precise data are demanded.

This work presents a finite element method (FEM) applied for a SAW device containing a diamond layer. We calculate the frequency response of such a structure in the sagittal plane and determine the parameters such as mode depth penetration for fundamental or harmonics modes. The dependence of the harmonics mode on the depth penetration for the AlN/diamond structure is analysed. After a description of the model, we present the obtained results for a layered structure of AlN/ diamond.

2. Model description

A general FEM modelisation is described for the AC steady state analysis of two-dimensional piezoelectric devices. This method is applied to layered surface acoustic wave structures. Assuming linear material and steady state sinusoidal time dependence, the quasi-static equations for the modeling of piezoelectric devices are Newton's law, Gauss's law and the constitutive relations. More details on the

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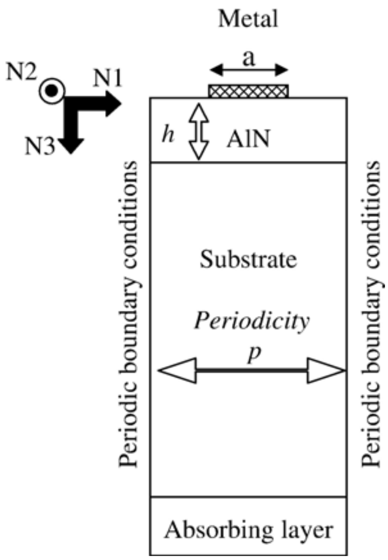

Fig. 1. Schematic representation of the studied structure in the model.

theoretical aspect are found in Refs. [8–10]. In this two-dimensional problem, we neglected the diffraction effect in the N2 direction (Fig. 1). Consequently no variation is permitted in the N2 direction (Fig. 1) and all the derivatives are equal to zero. As we are interested in harmonic response of the device, the governing differential equations which define the mechanical and electrical properties in the volume have to be established for the amplitudes of the mechanical displacement u_i (only in the N1 and N3 directions, Fig. 1) and the electrical scalar potential Φ in Eqs. (1a) and (1b).

$$\begin{cases} \sum_{j,k,l} C_{ijkl} \dfrac{\partial^2 u_j}{\partial x_j \partial x_i} + \sum_{j,k} e_{kij} \dfrac{\partial^2 \Phi}{\partial x_j \partial x_k} = \rho \dfrac{\partial^2 u_i}{\partial^2 t} & \text{(a)} \\ \sum_{k,l} e_{ikl} \dfrac{\partial^2 u_l}{\partial x_j \partial x_k} - \sum_{k} \varepsilon_{ik} \dfrac{\partial^2 \Phi}{\partial x_i \partial x_k} = 0 & \text{(b)} \end{cases} \tag{1}$$

S_{ij} Strain; T_{ij}: Stress; E_k: Electric field; D_i Dielectric displacement; Φ: Electric potential; C_{ijkl}: elastic constant; e-: piezoelectric constant; ρ: Density; ε_{ij}: Dielectric Permittivity; u_i: Mechanical displacement.

Besides these two sets of linear equations, we further evaluate integral quantities such as the electrical input impedance characterizing our piezoelectric device. The input impedance of a piezoelectric transducer also reveals all device resonances and anti-resonances. The resonances are the natural frequencies for short-circuited electrodes, while the anti-resonances are those for open-circuit conditions. To compute the electrical input impedance of a piezoelectric transducer with finite elements, the transducer has to be excited by a harmonic frequency and the integral calculation results can be used to quantify the mechanical and the electrical responses for example, the displacement of a region of interest, e.g., the surface of the device for Rayleigh waves. With those results the propagation mode is easy to determine by counting the number of nodes of the wave for the N3 displacement direction. The number of nodes gives the harmonic order of the propagating wave. Although the model can treat intrinsic material losses as imaginary parts of the physical constants, these leakage sources have been neglected in this work because almost no data are available for AlN or diamond. Nevertheless, these losses are assumed to be one of the principal device leakage source. The only leakage phenomena that can occur are then related to wave radiation into the bulk, which is absorbed by an additional layer in the model. This absorbing layer avoids the wave reflection from the backside of the sample in our model. Using the material constants given in Table 1, the model provides the electrical and the mechanical deformations of the layered structure. We assume a constant polarisation of 1 V on the aluminium electrode, which has a thickness of 150 nm. The metallization lateral (a) size is a 4 μm and the periodicity (p) is fixed at 12 μm. AlN thickness (h) was fixed at 5.2 μm in order to compare our result to previously published results.

Table 1

		AlN	Diamond
Elastic constants (10^{11} N/m^2)	C_{11}	3.45	11.5
	C_{12}	1.25	0.85
	C_{13}	1.20	0.85
	C_{33}	3.95	11.5
	C_{44}	1.18	5.37
Piezoelectric constants (C/m^2)	e_{15}	−0.48	–
	e_{31}	−0.58	–
	e_{33}	1.5	–
Relative dielectric constants (10^{-11} F/m)	ε_{11}	8	5.04
	ε_{33}	9.5	5.04
Mass density (10^3 kg/m^3)	ρ	3.26	3.515

3. Results

We can extract from the model the frequency response of the device. This typical result is characteristic of the waves that can

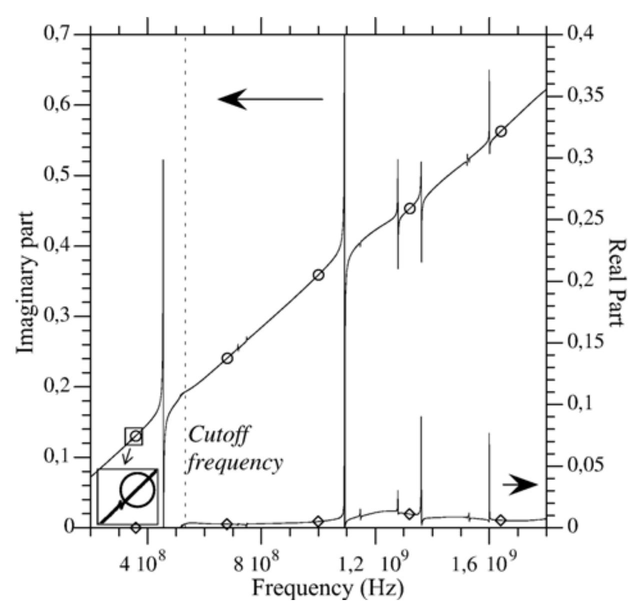

Fig. 2. Admittance response for the AlN/diamond structure, the periodicity p=12 μm (corresponds to a wavelength of 24 μm) and the AlN thickness h=5.2 μm and a=4 μm.