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FEM simulation of AlN thin layers on diamond substrates for high frequency SAW devices

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ABSTRACT

AlN/Diamond structure is very promising for high frequency acoustic wave devices. In this paper, a comprehensive investigation of AlN/Diamond structure is presented using finite element method. The phase velocity and the coupling coefficient of the first two modes of SAWs for the AlN/Diamond structure are numerically analyzed and compared to experimental data. Close agreement between experimental and numerical results is obtained. Results show that the mode 1 (Sezawa mode) exhibits the largest coupling coefficient of 1.28% associated with a phase velocity of 9500 m/s. Additionally, the temperature coefficient of frequency (TCF) and the reflection coefficient (r) are studied. The simulation results show that for a zero TCF, a high phase velocity of 10,800 m/s associated with a coupling coefficient of 0.5% can be obtained. These results demonstrate that the AlN/Diamond structure can be used to design wide-band and temperature-compensated SAW devices. The dependence of SAW devices performance with the electrode height, metallization ratio and mass-loading is also investigated.

1. Introduction

With the development of high-frequency and high-speed communication systems in the past decade, there is an increasing demand for surface acoustic wave (SAW) devices with higher frequencies. To extend the upper limitation of the operating frequency, high-velocity materials are required. Diamond is an attractive non piezoelectric material for high-frequency surface acoustic wave (SAW) devices due to its having the highest SAW velocity among all materials around 11,000 m/s with the small linear thermal expansion coefficient and TCF of around −1 ppm/C and −5 ppm/C, respectively [1]. Therefore, diamond is of particular interest for use in the design of gigahertz-band SAW devices recently. To induce high-velocity SAW, diamond has to be combined with the piezoelectric film, such as aluminum nitride (AlN) or zinc oxide (ZnO) which has been deposited on diamond [2,3,4]. AlN is the fastest piezoelectric materials among those that can be grown in thin film form: compared to ZnO, for example, AlN films show higher surface acoustic wave (SAW) velocity (5607 m/s as opposed to 2682 m/s), higher hardness (17.7 GPa as opposed to 4.7 GPa) and slightly lower electromechanical coupling coefficient K^2 (0.3% as opposed to 0.97%). The AlN resistance to high temperature and to caustic chemicals makes it the ideal candidate for the development of electro acoustic devices able to survive to harsh environment [5,6].

The AlN/Diamond structure has been investigated by many researchers [7,8,9,10,11]. The dispersion characteristics of SAWs with various film thicknesses have been theoretically and experimentally investigated. The results indicated that mode 1 has the largest coupling coefficient of 1.25%, which is associated with a phase velocity of 10,800 m/s at the optimal piezoelectric film thickness-to-wavelength ratio of 0.3 [7,11].

In the design of a layered SAW device, besides the need for a high velocity, high coupling coefficient, both temperature stability and high reflectivity are also equally important. Those parameters are affected by the geometrical parameters of SAW devices. Therefore, numerical studies using FEM are essentially required to optimize the performance of an AlN/Diamond structure.

This work presents a finite element method (FEM) applied for a SAW device containing a diamond layer. We calculate the SAW properties, including phase velocity, coupling coefficient, TCF and reflection coefficient, of mode 0 and mode 1 in the IDT/AlN/Diamond structure. Temperature-compensated AlN/Diamond structure with different thicknesses of piezoelectric film is numerically investigated. Also, the dependence of SAW devices performance with the electrode height, mass-loading and metallization ratio is studied.

2. Simulation methodology

The quasi-static equations for modeling piezoelectric devices are Newton's law, Gauss's law and the constitutive relations. Further details on the theoretical aspects are discussed in [12,13,14]. SAW propagation is governed by differential equations that must be solved along with design problems, including the geometric complexity of the device, the material properties, and the boundary conditions. The FEM provides

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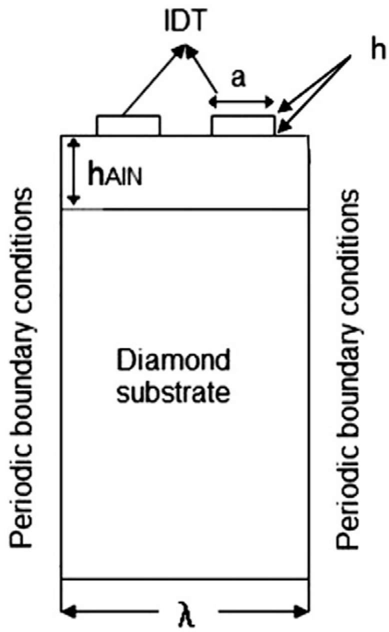

Fig. 1. Schematic representation of the studied structure in the model.

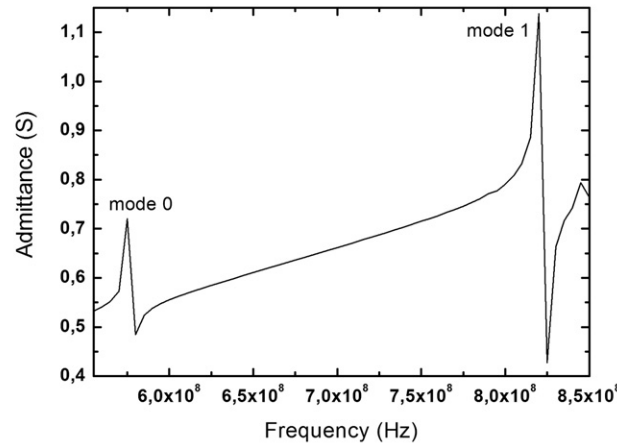

Fig. 2. Imaginary part of admittance response for the AlN/diamond structure with the periodicity p = 8 μm (corresponds to a wavelength of 16 μm) and the AlN thickness h_{AlN} = 2.54 μm.

numerical solutions defined by associated differential equations. The relation between the stress (T), strain (S), electric field (E), and electric displacement (D) of piezoelectric materials is given by the piezoelectric Eqs. (1) and (2) as follows [15]:

$$T_{ij} = c^E_{ijkl} S_{kl} - e_{kij} E_k \tag{1}$$

$$D_i = e_{ikl} S_{kl} + \varepsilon^S_{ij} E_k \tag{2}$$

where T_{ij} represents the stress vector, c_{ijkl} is the elasticity matrix (N/m^2), e_{ijk} is the piezoelectric matrix (C/m^2), ε_{ij} is the permittivity matrix (F/m), E_k is the electric field vector (V/m), S_{kl} is the strain vector, and D_i is the electrical displacement (C/m^2). The degrees of freedom (dependent variables) are the global displacements u_1, u_2, and u_3 in the global x, y, and z

Table 1
Elastic constants, mass densities, piezoelectric constants e $_{ij}$, and dielectric permittivities used for simulations [17,18].

	Materials		TEMPERATURE	Coefficients
Symbol	AlN	$Diamond_3$	AlN	Diamond
Density (kg/m^3)			(10^{-4}/°C)	
ρ	3260	3515	−14.69	−3.6
Elastic constants (GPa)			(10^{-4}/°C)	
C_{11}	34.5	115.8	0.8	−0.14
C_{12}	12.5	8.5	1.8	−0.57
C_{13}	12	–	1.6	–
C_{33}	39.5	–	1	−0.14
C_{44}	11.8	53.7	0.5	−0.125
Piezoelectric constants (C/m^2)			(10^{-4}/°C)	
e_{15}	−0.48	−0.45	–	–
e_{31}	−0.58	−0.51	–	–
e_{33}	1.5	1.22	–	–
Dielectric permittivitie (10^{-11} F/m)			(10^{-4}/°C)	
ε_{11}	8	7.41	–	–
ε_{33}	9.5	7.82	–	–
Thermal expansion coefficient (ppm/°C)				
α_{11}			5.27	1.2
α_{33}			4.15	1.2

directions. The electric potential V can be obtained by solving the Newton and Maxwell equations related to (1) and (2):

$$\rho \frac{\partial^2 u_i}{\partial t^2} = C_{ijkl} \frac{\partial^2 u_l}{\partial x_j \partial x_l} + e_{kij} \frac{\partial^2 \phi}{\partial x_j \partial x_l} \tag{3}$$

$$e_{jkl} \frac{\partial^2 u_l}{\partial x_j \partial x_l} - \varepsilon_{jk} \frac{\partial^2 \phi}{\partial x_j \partial x_l} = 0 \tag{4}$$

i, j, k, l = 1, 2 and 3.

Rayleigh SAW propagates over the surface of the piezo-substrate and amplitude decays exponentially with the depth of the substrate. Most of the energy is concentrated near the surface of the substrate. The displacement has both surface normal and surface parallel components in the direction of the wave propagation. In this case, there is no displacement in parallel transverse direction of the wave propagation. These features enable us to model the SAW resonator device in 2 dimensions (2D) and with only few wavelengths depth of the piezo substrate. The infinite numbers of IDT fingers are modeled using periodic boundary conditions.

The boundary conditions require that the acoustic displacements and stresses be continuous at the AlN-diamond interface and the stress-free surface is assumed on both sides of the structure. In addition, the electric potential and the normal component of electric displacement must be continuous at the interface for an electrically free surface [16]. For a metalized (thin metal film) surface, the electric potential is equal to zero.

A schematic of the layered structure, which consists of a Diamond substrate, an AlN film, and IDTs, is presented in Fig. 1. The thicknesses of the AlN film are denoted by h $_{AlN}$, and λ is the wavelength of the SAW.

The material constants of AlN film and Diamond substrate presented in Table 1 are taken from reports by [17,18].

We can extract from the model the frequency response of the device. Fig. 2 shows the harmonic admittance of the implemented structure, providing a quite easy identification of the excited modes. The frequency response (Fig. 2) presents several peaks in the range 500 MHz–850 MHz. Those peaks correspond to mode 0 and mode 1 surface acoustic wave.

In order to determine precisely the acoustic wave propagation properties in this structure we have plotted in Fig. 3 the shape of the first four observed acoustic surface eigenmodes. The first modes have a magnitude higher displacement caused by the particle displacement close to the free surface. These modes represent the four stopband edges of the first two Rayleigh waves. Each propagating mode has two resonance