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Investigation of properties of surface acoustic waves generated by periodically patterned ZnO on silicon substrate

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ABSTRACT

The paper presents the characteristics of vertically polarized surface waves generated in silicon substrate by acoustic coupling of bulk waves excited in a periodically patterned ZnO film on silicon. The finite element simulations are performed on the proposed patterned-ZnO/Si structure and vertically polarized modes in silicon are found to be dominant in the frequency dependent analysis. The generated modes in silicon are concentrated near the surface within a wavelength depth and exhibit surface wave properties. Dispersion curves of phase velocity and coupling coefficient for the surface modes are reported. The results indicate high electromechanical coupling coefficient of 6.4% as well as high phase velocity of 5332 m/s for the surface mode generated in silicon owing to the acoustic coupling of the first order bulk mode in ZnO pattern observed at ZnO height to wavelength ratio of 0.19.

1. Introduction

Surface acoustic wave (SAW) devices are widely used in wireless and telecommunication systems. High performance SAW devices like SAW filters, correlators and delay lines, are used for signal processing and sensing applications with a wide range of frequencies. Most of these devices are fabricated over piezoelectric substrates like lithium niobate, lithium tantalate, and quartz and their operating frequency is determined by electrode dimensions and substrate velocity [1]. The surface waves are generated by the transduction of electrical to mechanical energy using interdigital transducers (IDT). SAW devices can also be implemented over non-piezoelectric substrates by using piezoelectric overlays and IDT for applications like, high frequency devices and integration with CMOS circuitry [2,3]. Surface waves are also used in nondestructive testing of materials where SAWs are generated by mode conversion using bulk acoustic wave transducers [4]. Since, silicon is the widely used material for microelectromechanical systems and integrated circuits fabrication, implementing SAW devices on silicon can result in monolithic compact devices with low acoustic losses and high performance [3]. In general, *c*-axis oriented ZnO is preferred for implementing SAW devices on silicon due to its high coupling coefficient and compatibility with CMOS process desirable for fabrication of low loss and small size devices on Si [5]. However, the conventional layered structures exhibit a trade-off between phase velocity and electromechanical coupling coefficient (K^2). The insertion loss of layered devices depends on the quality of thin film which is difficult to reproduce for mass production [6,10].

In general, mutual transformation occurs between surface acoustic waves and bulk acoustic waves (BAW) at periodic grooves and irregularities [7]. The incident BAWs at the interface of periodic grooves and substrate are transformed into longitudinal or transversely polarized surface waves along the direction of propagation [8]. In the current study, we propose periodically patterned ZnO between fingers of IDT to implement SAW resonators on silicon. The structure resembles periodically placed bulk acoustic wave resonators excited laterally, as depicted in Fig. 1(a). The bulk modes generated in the ZnO pattern acoustically couple to silicon substrate can result in generation of surface waves in silicon. The coupling between transducer and substrate depends on the mode generated in ZnO and characteristic impedances of ZnO and silicon. The acoustic power transmission and reflection coefficients [9] of acoustic waves with normal incidence at the interface of ZnO pattern and silicon are given by,

$$T = \frac{4Z_{Si}Z_{ZnO}}{(Z_{ZnO} + Z_{Si})^2}; \quad R = \left(\frac{Z_{ZnO} - Z_{Si}}{Z_{ZnO} + Z_{Si}}\right)^2$$

where Z_{ZnO} and Z_{Si} are the characteristic impedances of ZnO and silicon respectively.

The energy flux of BAW generated in ZnO and two SAWs generated along the silicon surface in opposite directions are given by [8]

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$$P_{BAW} = \rho_{ZnO} v_{BAW} \omega^2 N |A_{BAW}|^2; \quad P_{SAW} = \frac{2\rho_{Si} v_{SAW}^2 \omega^2 |A_{SAW}|^2 T}{\alpha}$$

where N is the number of ZnO structures, A is the amplitude of acoustic wave, and α is the decay factor of wave propagation into depth. In this work, we present the characteristics of SAWs generated in the proposed device obtained using finite element method (FEM) and the results are compared with conventional layered ZnO/Si structure.

2. Model description

In general, SAW device features a large number of uniform interdigital electrodes and their periodic nature allows us to model the device using half spatial period of IDT ($\lambda/2$) using periodic boundary conditions with sign inversion of variables to the boundaries [10]. Three dimensional (3D) model is considered for the analysis of surface modes generated in the composite structure. Uniform IDT with metallization ratio of 0.5 is patterned over the (100) oriented silicon substrate and overlaid ZnO is patterned along the aperture of IDT to fill spaces between fingers, as depicted in Fig. 1(b). The (002) oriented ZnO with c-axis along the sagittal plane is chosen due its maximum electromechanical coupling for the waves propagating along c-axis [11]. Perfectly matched layer (PML) is considered at the bottom of the silicon substrate as an absorbing boundary to eliminate the unwanted reflections from bottom surface and fixed boundary condition is applied to the bottom surface of PML. We assume electrode width of 2 μm and 150 nm thickness with pitch 4 μm and the material properties of ZnO, silicon, and aluminum used in the simulation are adapted from [12]. A potential of 1 V is assumed for the IDT to obtain harmonic admittance of the proposed structure using frequency dependent analysis. In the simulations, the effect of mechanical properties of aluminum and silicon are taken into account. We considered exactly vertically patterned ZnO for theoretical study because of its high reflectivity and high coupling coefficient compared with triangular or trapezoidal shapes [7]. From the fabrication perspective, ZnO can be patterned with exact 90° angle with silicon surface and its process is described elsewhere [16]. From Eigen mode analysis, the frequency of generated surface mode is obtained and its phase velocity (v) is calculated using $v = f\lambda$, where λ is the wavelength of IDT.

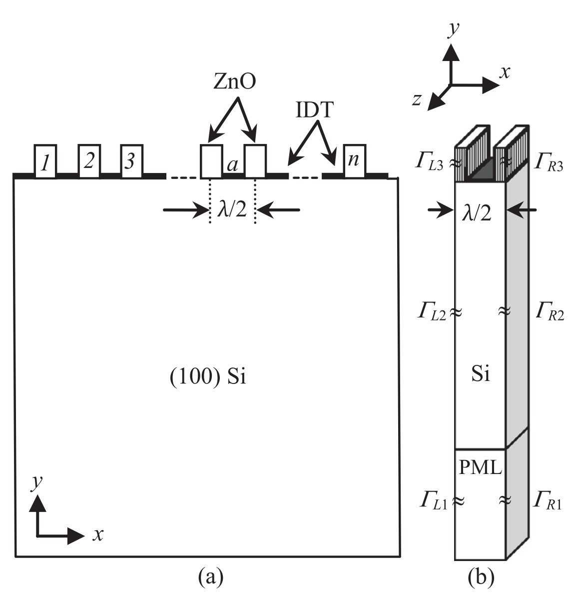

Fig. 1. (a) Schematic of the device structure and (b) geometry used with periodic boundary conditions in simulations.

The electromechanical coupling coefficient (K^2) of the proposed structure is calculated using $K^2 = 2(v_f - v_m)/v_f$ [9,13], where v_f and v_m are the SAW phase velocities obtained when the interface boundary between ZnO and silicon containing IDT is electrically free and shorted, respectively.

3. Results and discussion

In this section, we discuss the characteristics of surface waves generated in the silicon substrate and polarization at the ZnO–silicon interface for the device structure shown in Fig. 1(b). Since wavelength λ and ZnO height h are two independent parameters, it is convenient to use the normalized parameters $f\lambda$ and h/λ for device characteristics.

The harmonic admittance (HA) and normalized displacement plots of surface modes generated in the proposed structure (Fig. 2) are obtained at $h/\lambda = 0.19$ at which we have observed high electromechanical coupling coefficient as well as high phase velocity in the dispersion characteristics as summarized in Table 1. Three surface modes are observed from the HA plot and normalized displacement plots. The surface modes with predominant displacement along y are considered as vertically polarized (VP) modes and the modes with predominant displacement along z are consider to be shear horizontally polarized (SH) modes. From the displacement plots in Fig. 2, the displacements for SH surface modes are insignificant compared to the displacements of VP modes in case of periodically patterned (002) ZnO, which confirms the insignificant existence of shear polarized modes in the proposed structure as the shear horizontal coupling is minimal along c-axis in ZnO [11].

Fig. 3 shows, the normalized x and y displacement profiles of vertically polarized SAW modes generated in the patterned-ZnO/Si structure at h/λ of 0.19. The displacements are normalized with respect to the maximum y displacement in silicon. The x displacement profiles in Fig. 3(a) and (c) depict the generation of transverse BAW in ZnO pattern and y displacement profiles in Fig. 3(b) and (d) show dominant normal component in silicon at the IDT interface. It explains the generation of VP SAWs due to bulk transverse modes generated in periodic ZnO patterns. From Fig. 3(e) and (f), the dominant normal component at ZnO silicon interface is due the acoustic coupling of longitudinal BAW generated in ZnO and the displacement profile resembles Rayleigh waves. Plessky et al., reported similar result with periodic structure of bulk acoustic wave resonators formed by patterning piezoelectric material only under IDT [17]. In the proposed patterned-ZnO/Si structure, as the cross fields in ZnO structure are dominant compared to inline fields (along c-axis), hence transverse BAW is dominant over longitudinal BAW in ZnO pattern and the dominant surface modes observed in HA plot from Fig. 2 are excited by the transverse BAW in ZnO. The VP surface modes generated in silicon by transverse and longitudinal bulk waves in ZnO are referred as VP_T and VP_L respectively. The phase velocity and K^2 characteristics of the surface modes generated in the proposed device with respect to ZnO height to wavelength ratio are as follows.

3.1. Characteristics of SAWs generated by transverse modes in ZnO

The SAW phase velocity dispersion characteristics for the first five vertically polarized SAW modes generated by the transverse waves in proposed structure with respect to ZnO height to wavelength ratio (h/λ), are shown in Fig. 4. From the dispersive curves, we observed that with increase in height of ZnO the phase velocity of generated SAW decreases rapidly due to the decrease in frequency of bulk mode in ZnO structure. The first higher order transverse mode in ZnO results in generation of VP_{T1} in the structure at