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Surface Acoustic Wave Velocity in Single-Crystal AlN Substrates

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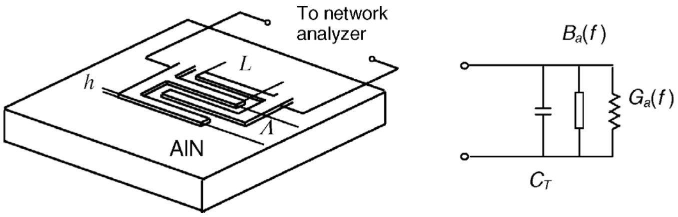
***Abstract*—The surface acoustic wave velocity has been measured on *a*-plane (*c*-propagation) and *c*-plane oriented bulk aluminum nitride (AlN) single crystals using the S_{11}-parameter method in the frequency range 160–360 MHz. The SAW velocity is 5760 m/s for both orientations. From comparison of this value with the simulations using various elastic constants of AlN available in literature, we estimated the elastic constant c_{44} to be 122 ± 1 GPa.**

I. Introduction

Piezoelectric single crystal aluminum nitride (AlN) is a very attractive material for applications in surface acoustic wave (SAW) technology. A high acoustic wave velocity is a very important advantage of AlN for a high-frequency SAW operation, as compared to other piezoelectric materials. However, the calculations of the SAW velocity based on material parameters of AlN available in literature yield values that vary by more than 10% in magnitude. A much better accuracy is required for the design of SAW devices, such as filters, resonators, oscillators, etc. Recent progress in the growth of large bulk AlN single crystals [1] makes experimental studies of SAW properties in such substrates possible [2]. In this paper, we report on the direct measurements of the SAW velocity in bulk single crystal AlN and compare the experimental values with those calculated using material parameters available in the literature.

II. Methods



(a) (b)

Fig. 1. Experimental configuration (a) and equivalent circuit of the interdigital transducer (b).

The velocity of a surface acoustic wave propagating on the piezoelectric substrate is found according to the analytical procedure described in the literature (see, e.g., [3]). We have calculated the SAW velocity V_f on a free surface of hexagonal AlN crystal using elastic constants reported by various authors [4]–[14] (see Table I). In the experimental part of Table I, the constants of McNeil *et al.* [13] were extracted from single crystal AlN and others were from AlN films. Other material parameters used in the calculations are given in Table II. Our numerical simulations show that variations of piezoelectric and dielectric constants have only a minor effect on the calculated velocity values. It also should be noted that the constants of [10], due to the evaluation method, are "stiffened", i.e., they reflect the piezoelectric contribution. Therefore, in order to not account for the piezoelectric effect twice, the piezoelectricity was excluded in our calculations for this particular case. One can see from Table I that the various sets of elastic constants lead to the differences in V_f values up to 14%.

III. Results

We have measured the SAW velocity in bulk, single crystal AlN using the S_{11}-parameter method. The *c*- and *a*-plane oriented AlN single crystals were grown by the sublimation-recondensation technique [1]. The oxygen impurity concentration of oxygen has been found by secondary ion mass spectroscopy (SIMS) measurements to be in the range of 10^{18} cm^{-3}. A SAW interdigital transducer (IDT) made of Al film of thickness h was deposited on the sample surface and connected to the Agilent 4396B network analyzer (Agilent, Palo Alto, CA) for the measurements of the reflection coefficient S_{11}. The SAW propagation direction was arbitrary on the *c*-plane and along *c*-axis on the *a*-plane. The measurements were performed using various transducers with different periods Λ, numbers of periods N, and aperture lengths (see Table III). The experimental configuration and the equivalent circuit of the transducer are shown in Fig. 1. Fig. 2 shows an example of the IDT radiation conductance G_a and motional susceptance B_a dependencies on frequency f extracted from the

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Manuscript received December 10, 2003; accepted June 24, 2005. The work at RPI was supported by Crystal IS under a subcontract from DARPA (Project Manager Dr. Edgar Martinez and monitored by John Blevins at AFRL, contract F33615-02-C-5417). The work at SET, Inc. was partially supported by NASA under contract NAG5-10322.

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TABLE I
Elastic Constants of AlN and Relevant SAW Velocities.

	Elastic constants (GPa)					V_f (km/s)	
Reference	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c-plane	a-plane, c-prop.
Theoretical							
[4]	464	149	116	409	128	5.93	5.93
[5]	398	142	112	383	127	5.82	5.84
[6]	396	137	108	373	116	5.62	5.63
[7]	380	114	127	382	109	5.46	5.48
[8]	398	140	127	382	96	5.21	5.21
[9]	369	145	120	395	96	5.20	5.21
Experimental							
[10]	411	149	99	389	125	5.79	5.79
[11]	410	140	100	390	120	5.73	5.74
[12]	345	125	120	395	118	5.59	5.63
[13]	360	122	123	410	116	5.59	5.62
[14]	424	122	166	353	123	5.65	5.65

TABLE II
Material Parameters Used for SAW Velocity Calculations.

AlN					
Piezoelectric constants [15] (C/m^2)			Dielectric constants [16]		Mass density [17] (10^3 kg/m^3)
e_{33}	e_{31}	e_{15}	$\varepsilon_{11}/\varepsilon_0$	$\varepsilon_{33}/\varepsilon_0$	ρ
1.39	-0.57	-0.29	8.5	8.5	3.26

Al		
Elastic constants [19] (GPa)		Mass density [19] (10^3 kg/m^3)
c_{11}	c_{44}	
111	25	2.7

TABLE III
Parameters of Interdigital Transducers and Measured Values of SAW Velocity.

Sample orientation	c-plane					a-plane
SAW propagation	Arbitrary				Normal to that at left	c-axis
IDT period (acoustic wavelength), Λ (μm)	16	16	16	24	36	24
Number of finger pairs, N	90	90	70	70	70	62
Aperture length, L (mm)	1.3	1.3	0.5	0.5	0.5	0.5
Al film thickness, h (μm)	0.1	0.1	0.2	0.2	0.1	0.1
Center frequency (MHz)	358.5	358.5	357.5	239.2	159.7	239.2
SAW velocity (m/s)	5736	5736	5720	5741	5749	5741

S_{11} parameter measurements. The measured dependencies were fitted to those calculated using the relation [18]:

$$G_a(f) = G_0 \left(\frac{\sin X}{X} \right)^2, \tag{1}$$

$$B_a(f) = G_0 \frac{\sin 2X - 2X}{2X^2}, \tag{2}$$

where $X = N\pi\,(f - f_0)/f_0$, and $G_0 = 8 f_0 K^2 C_T N L$. The fitting parameters were the transducer center frequency f_0 and the product $K^2 C_T$, where K^2 is the electromechanical coupling coefficient, and C_T is the transducer electrode-overlap capacitance. The SAW velocity is found from the relation $V = f_0 \Lambda$, where the transducer period Λ is equal to the acoustic wavelength. The obtained values of V are given in Table III.

It should be noted that the measured SAW velocity is slightly different from that on the free crystal surface due to the presence of the transducer metal electrodes. A metal film on the surface of a piezoelectric substrate affects the

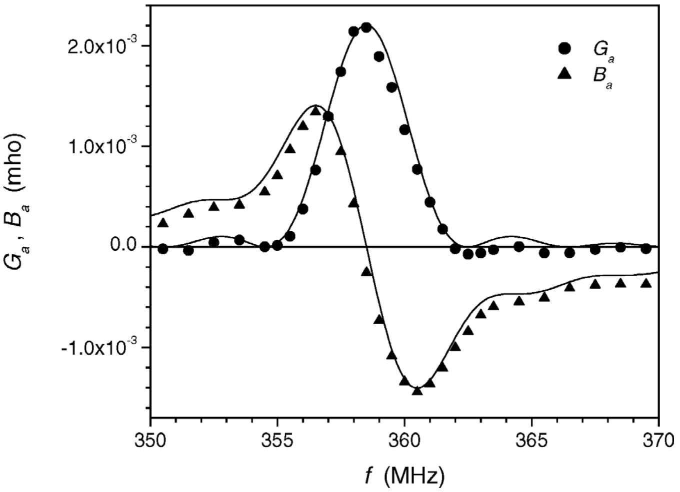

Fig. 2. Radiation conductance G_a and motional susceptance B_a of SAW interdigital transducer versus frequency on *c*-plane of bulk AlN crystal. Acoustic wavelength 16 μm. Dots and triangles, experiment; lines, theory.

SAW velocity by the mechanical loading and by the short-circuiting of electric fields [19]. We have plotted, in Fig. 3, the measured SAW velocity against the product kh, where $k = 2\pi/\Lambda$ is the acoustic wave number. The dependence $V(kh)$ can be approximated by a linear function, the slope of which is in good agreement with simulations for the Al film-on-AlN substrate structure (with the Al conductivity neglected). Hence, the observed decrease in V with increasing kh can be attributed to the mechanical loading, which is eliminated by extrapolating the $V(kh)$ dependence to $kh = 0$. The effect of short circuiting by the film conductance leads to the SAW velocity drop according to the relation:

$$\frac{\Delta V}{V} = \frac{K^2}{2}. \tag{3}$$

The free-surface velocity can be restored from the velocity value on the half-metallized surface at $kh = 0$ by adding the amount $(1/4)\,K^2V$. The electromechanical coupling coefficient K^2 for SAWs in single-crystal AlN substrates is 0.47% for *a*-plane *c*-propagation, and 0.11% for *c*-plane [15]. Consequently, we obtain the free-surface SAW velocity 5.76 ± 0.01 km/s both for *a*-plane (*c*-propagation) and *c*-plane orientations. One can see from Table I that the elastic constants experimentally determined from Brillouin scattering measurements in AlN single-crystal platelets [10] and SAW measurements in AlN thin films on sapphire substrates [11] give the best agreement (within ±0.5%) between calculated and our measured SAW velocity values. A slightly larger discrepancy (about 1%) is obtained using the theoretically calculated elastic constants from [5]. Other sets of elastic constants yield larger differences, from 2 up to 10%, from our value. Our numerical simulations show that the SAW velocity is very sensitive to the changes in the c_{44} value and is a weak function of other elastic constants. Thus the calculated SAW velocity can be fitted to the measured value by adjusting the c_{44} value.

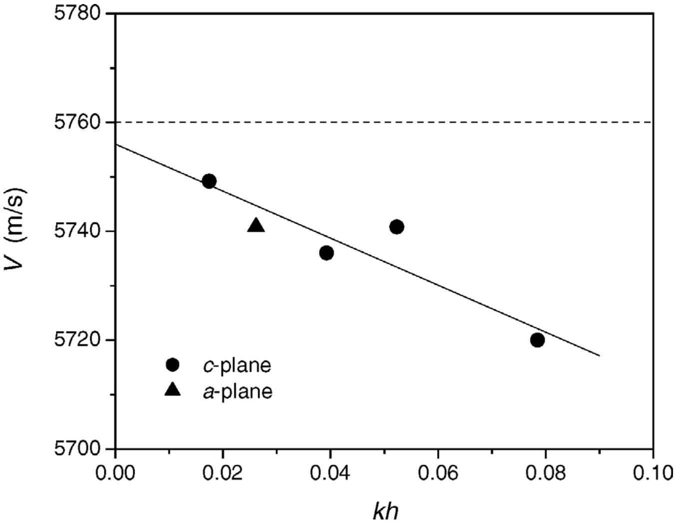

Fig. 3. SAW velocity in bulk AlN versus SAW wave number-Al film thickness product kh. Dots, experiment; solid line, slope of $V(kh)$ dependence due to mechanical loading of AlN surface by Al film; dashed line, free-surface velocity.

The SAW velocity value calculated using any set of the elastic constants from [5], [10], [11] becomes equal to our experimental V_f value if the c_{44} value is adjusted in the range 122 ± 1 GPa. Therefore, our SAW velocity studies yield a definite value of c_{44} with good accuracy.

IV. CONCLUSIONS

We have measured the SAW velocity for the *a*-plane *c*-propagation and *c*-plane oriented single crystal, bulk AlN. The velocity value is 5.76 km/s for both orientations. We compared our velocity value with the values calculated using elastic constants available in the literature and estimated the consistency of different c_{ij} sets with our results. The elastic constant c_{44} of AlN crystal estimated from our measurements is 122 ± 1 GPa.

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