Electromechanical coupling coefficient for surface acoustic waves in single-crystal bulk aluminum nitride

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The electromechanical coupling coefficient K^2 for surface acoustic waves propagating on c and a surfaces of bulk AlN single crystals has been measured using the S_{11}-parameter method in the frequency range of 160–360 MHz. The extracted values of K^2 are 0.11% and 0.47% for the c and a surfaces, respectively. By fitting our experimental data to our numerical simulation results, we have estimated piezoelectric constants, which are in a reasonable agreement with literature data. Our results are consistent with the negative sign of the e_{15} constant. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1755843]

Piezoelectric properties, high sound velocity, and capability to withstand high temperatures and chemically aggressive environments make aluminum nitride a very attractive material for surface acoustic wave (SAW) applications, such as SAW filters, resonators, and sensors. Up until now, most of work in this area has been done using AlN films deposited on different foreign substrates by sputtering, chemical vapor deposition, or molecular-beam epitaxy techniques.[1–3] The progress in material growth (see, e.g. Ref. 4) enabled us to perform, the experimental studies of SAW propagation in bulk AlN single crystals.[5] The knowledge of the electromechanical coupling coefficient, K^2, is of primary importance for the SAW device design. The electromechanical coupling coefficient can be calculated provided the material parameters, such as piezoelectric, elastic, and dielectric constants of the crystal, are known. However, the data on piezoelectric constants of AlN available from literature are controversial. Aside from the disagreement in numerical values, various authors reported different signs for the piezoelectric constant e_{15}. In the present letter, we report on the results of the electromechanical coupling coefficient measurements for SAWs propagating on a- and c-cut single crystal, bulk aluminum nitride. From the comparison of our experimental K^2 values to those numerically simulated, we estimate the magnitudes of piezoelectric constants of AlN and determine the sign of e_{15}.

The electromechanical coupling coefficient for a SAW propagating in the piezoelectric crystal is defined as

$$K^2 = 2\,\frac{V_f - V_m}{V_f}, \tag{1}$$

where V_f and V_m are the SAW velocities for free and electrically short-circuited surfaces of the crystal, respectively.[6] The velocities are found by solving the system of equations (see, e.g., Ref. 7):

$$\rho\,\frac{\partial^2 u_j}{\partial t^2} - c_{ijkl}\frac{\partial^2 u_k}{\partial x_i \partial x_l} - e_{kij}\frac{\partial^2 \phi}{\partial x_i \partial x_k} = 0, \tag{2}$$

$$e_{ikl}\frac{\partial^2 u_k}{\partial x_i \partial x_l} - \epsilon_{ik}\frac{\partial^2 \phi}{\partial x_i \partial x_k} = 0, \quad i,j,k,l = 1,2,3 \tag{3}$$

for relevant boundary conditions. Here, u_j are the components of elastic displacement and ϕ is the electric potential of the wave, c_{ijkl}, e_{ikl}, and ϵ_{ik} are the components of elastic, piezoelectric, and dielectric permittivity tensors, respectively, and ρ is the mass density.

We have calculated the electromechanical coupling coefficients using material parameters of AlN available from literature (see Tables I and II). We neglected a weak anisotropy of the dielectric constant.[2] It should be noted that a variation of elastic and dielectric constants in the range of values reported in literature did not much affect the results of the K^2 calculation. Piezoelectric constants e_{ij} and d_{ij} of AlN available from literature are given in Table II. They are related as $e_{ip} = d_{iq} c_{qp}$ and $d_{ij} = e_{ik} s_{kj}$, where the matrix of elastic

TABLE I. Material parameters of AlN used for K^2 calculation.

Elastic stiffness constants (GPa)[a]					Dielectric constant[b]		Mass density (10^3 kg/m^3)[c]
c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	ϵ_{11}/ϵ_0	ϵ_{33}/ϵ_0	ρ
410	140	100	390	120	8.5	8.5	3.26

[a]See Ref. 4.
[b]See Ref. 8.
[c]See Ref. 9.

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TABLE II. Piezoelectric constants of AlN and relevant values of electromechanical coupling coefficient for SAWs.

Reference		Piezoelectric constants e_{ij} (C/m^2)			K^2 (%)	
		e_{33}	e_{31}	e_{15}	c plane	a plane, c propagation
Tsubouchi *et al.*[a]		1.55	-0.58	-0.48	0.25	0.81
Our values		1.39 ± 0.22	-0.58 ∓ 0.23	-0.29 ± 0.06	0.11	0.47
		Piezoelectric constants d_{ij} (pm/V)				
		d_{33}	d_{31}	d_{15}		
Bernardini and	GGA	5.4	-2.1	2.9	0.09	0.05
Fiorentini[b]	LDA	6.4	-2.6	3.4	0.13	0.07
Our values		4.53 ± 0.86	-1.88 ∓ 0.57	-2.42 ± 0.50	0.11	0.47

[a]Experimental, Ref. 2.
[b]Theoretical, Ref. 10.

compliance constants s_{ij} is inverse to that of the elastic stiffness. Hexagonal AlN crystals have three independent piezoelectric constants. Full sets of the piezoelectric constants required for K^2 calculation have been evaluated experimentally from the SAW measurements in epitaxial AlN films on sapphire substrates[2] and calculated theoretically by two methods: Generalized gradient approximation (GGA) and local density approximation.[10] Other literature data on piezoelectric constants of AlN are incomplete and do not allow to perform the K^2 calculation. In particular, the sign of d_{15} was ambiguously determined in Ref. 11 and only absolute value of d_{15} was measured in Ref. 12. The two sets of piezoelectric constants[2,10] lead to the substantial differences in K^2 values, which might be attributed to different signs of the constant e_{15}. The K^2 value on the c plane is not much affected by the sign of e_{15}, whereas for the a plane, the predicted K^2 is much larger at $e_{15}<0$, and is very small at $e_{15}>0$. This controversy does not allow us to predict unambiguously the electromechanical coupling coefficient for SAWs in AlN from literature data but it can be resolved by direct experimental measurements.

We performed the measurements of K^2 for SAWs in bulk single-crystal AlN using the S_{11}-parameter method. The growth of AlN crystals was done using the sublimation–recondensation technique. The growth details can be found in Ref. 6. The c-plane-oriented sample had the approximate dimensions of $8\times4\times0.5$ mm^3. The a-plane-oriented crystal of a similar size was embedded in an AlN ceramic environment. A single Al film SAW interdigital transducer (IDT) has been deposited on the sample surface and connected to the network analyzer Agilent 4396B for the measurements of the complex reflection coefficient S_{11}. The equivalent circuit of

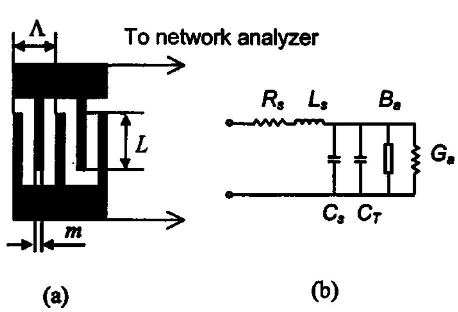

FIG. 1. Geometry (a) and equivalent circuit (b) of the IDT. Metallization ratio is defined as $\eta=2m/\Lambda$.

the SAW transducer[13] shown in Fig. 1 comprises the radiation conductance G_a, the motional susceptance B_a, and the static capacitance $C_T=C_1NL$, where C_1 is the finger-overlap capacitance per period and per unit length, N is the number of transducer periods, and L is the aperture length. In our measurements, we also accounted for the stray components: The ohmic resistance R_s of the electric connections and film electrodes, the inductance L_s of connecting wires, and the capacitance C_s of the header and bond pads. Parameters of the transducers used are given in Table III. An example of $G_a(f)$ dependencies extracted from the S_{11} measurements in the frequency range around the transducer center frequency $f_0=V/\Lambda$ is shown in Fig. 2. On the a plane, the SAW propagated along the c axis. For the c plane, the SAW propagation direction was arbitrary since the SAW properties in the basal plane of a hexagonal crystal are direction independent. The measured dependencies were fitted to those calculated using the relation[13]

$$G_a(f)=G_0\left(\frac{\sin X}{X}\right)^2, \tag{4}$$

where $X=N\pi(f-f_0)/f_0$, and $G_0=8f_0K^2C_1N^2L$, with the transducer center frequency f_0 and electromechanical coupling coefficient K^2 as fitting parameters. The measured value $C_1=79$ pF/m is in a good agreement with that calculated from the following expression[14]

$$C_1=2(6.5\eta^2+1.08\eta+2.37)(\epsilon/\epsilon_0+1), \tag{5}$$

using the dielectric constant $\epsilon/\epsilon_0=8.5$ and the mean metallization ratio for our transducers $\eta=0.45$. The K^2 values obtained for different frequencies and crystal orientations are plotted in Fig. 3. The mean K^2 value for the c plane is 0.11%. A much higher value $K^2=0.47\%$ is obtained for the a plane. Our values are somewhat lower than those previously reported for AlN films.[2]

Using Eqs. (1)–(3), we performed the numerical simulations of K^2 by varying values of piezoelectric constants to fit

TABLE III. Parameters of IDTs used in experiments.

Sample orientation SAW propagation direction	c-plane arbitrary			a plane c axis
IDT period, Λ (μm)	16	24	36	24
Center frequency (MHz)	358	239.2	159.7	239.2

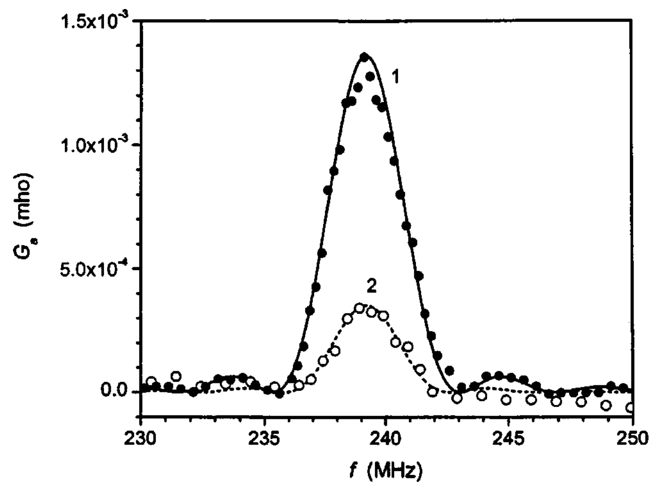

FIG. 2. Radiation conductance of SAW IDT on bulk AlN crystal as function of frequency at acoustic wavelength 24 μm; (1) *a* surface, *c* propagation and (2) *c* surface. Dots, experiment; lines, theory.

our measured K^2. From the measurements for the two orientations, *a* and *c* planes, the three piezoelectric constants cannot be extracted unambiguously. However, if one of the constants, e.g., e_{33}, is chosen, the other two are uniquely determined. The values of piezoelectric constants e_{31} and e_{15} found to yield $K^2=0.11\%$ and $K^2=0.47\%$ on *c* and *a* planes, respectively, at a given e_{33} value are plotted in Fig. 4. The reasonable range of e_{33} can be determined by observing that for wurtzite nitrides, the relations $|e_{31}|\leqslant 0.5e_{33}$ and $|e_{15}|\leqslant|e_{31}|$ hold, with the equality sign in both relations corresponding to an ideal wurtzite structure.[15] The obtained allowable values of piezoelectric constants e_{ij} and d_{ij} are shown in Table II. Our estimated range of magnitudes of the piezoelectric constants is in a reasonable agreement with rather scattered data of other authors. For example, d_{33} values ranging from 3 pm/V[16] to 6.72 pm/V[17] have been reported. Our results confirm that the sign of e_{15} in AlN is negative, just as the sign of e_{15} for II–IV group wurtzites CdS and ZnO.[15]

In conclusion, we have measured the electromechanical

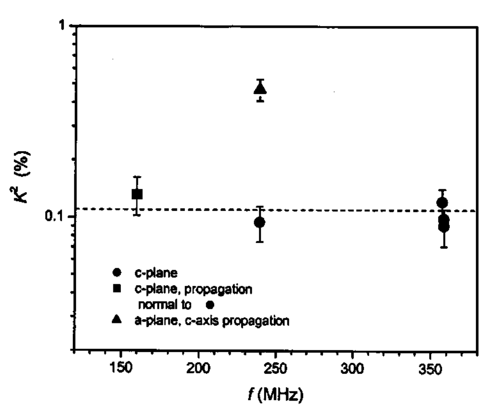

FIG. 3. Electromechanical coupling coefficient of bulk AlN extracted from radiation conductance measurements using different transducers listed in Table III. Dashed line shows average value for *c* plane.

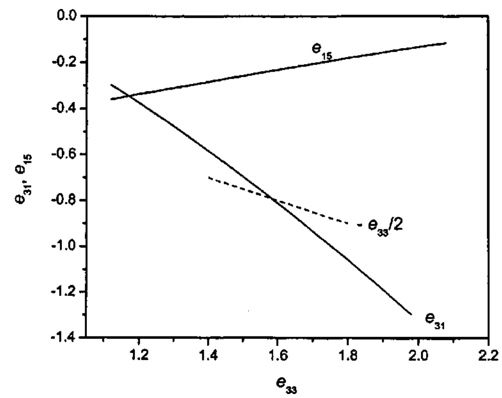

FIG. 4. Piezoelectric constants e_{33}, e_{31}, and e_{15} satisfying the condition $K^2=0.11\%$ and $K^2=0.47\%$ for SAWs on *c* and *a* surfaces of AlN, respectively.

coupling coefficients for SAWs propagating in bulk AlN single crystals in the frequency range from 160 to 360 MHz. The measured values are 0.11% and 0.47% for the *c* and *a* surfaces, respectively, revealing the advantage of *a*-cut crystals for SAW applications. By fitting our experimental results to our numerical simulation, we have estimated the allowable range of piezoelectric constants of AlN, which is in a reasonable agreement with rather scattered literature data. Our results confirm constant e_{15} is negative for AlN.

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