Pure Shear Bulk Acoustic Wave of the Oriented AlN

Sean Wu[1], Zhi-Xun Lin[2], Maw-Shung Lee[3], Ruyen Ro[4], and K. I Chen[1]
[1] Department of Electronics Engineering and Computer Sciences, Tung-Fang Institute of Technology, 110 Tung-Fung Road, Hunei Shiang, Kaohsiung 829, Taiwan, R.O.C.
[2] Department of Electrical Engineering, National Kaohsiung University of Applied Sciences, 415 Chien Kung Road, Kaohsiung 807, Taiwan, R.O.C.
[3] Department of Electronic Engineering, National Kaohsiung University of Applied Sciences, 415 Chien Kung Road, Kaohsiung 807, Taiwan, R.O.C.
[4] Department of Communication Engineering, I-Shou University, 1, Section 1, Hsueh-Cheng Rd., Ta-Hsu Hsiang, Kaohsiung County 840, Taiwan, R.O.C.

Abstract — Characteristics of bulk acoustic wave (BAW) propagating in (100)-, (002)-, (110)-, (200)-, (210)- and (300)-oriented AlN were investigated in this study. It was found the (002)-oriented AlN provided a pure longitudinal mode, while the (100)-, (110)-, (200)-, (210)- and (300)-oriented AlN supported a pure fast shear mode with the phase velocity 5867 m/s and the piezoelectric coupling constant (K^2) 2.45 %. The (100)-, (110)-, (200)-, (210)- and (300)-oriented AlN can be employed for the design of thin film acoustic wave resonator (FBAR) liquid sensor.

Introduction

Recently, lots of efforts have been made in the development of electro-acoustic resonators for the design of frequency control components in wireless communication systems. For a film bulk acoustic wave resonator (FBAR) device fabricated upon AlN film, the goal, in general, is to grow films with perfect c-axis orientation in order to excite optimally the longitudinal thickness mode [1-8].

In recent decades, substantial efforts have been made for the development of electro-acoustic resonators for sensing applications in liquid media. In a liquid medium, longitudinally polarized wave resonators show significant acoustic leakage into the liquid, which results in a substantial loss of resolution [9]. For immersed-sensor applications, the shear thickness mode does not produce any compressional motion in the liquid; thus, no energy leakage occurs [10-13]. For liquid sensing applications, FBAR devices which can excite stiffen, pure shear modes are promising candidates. In this study, the theoretical BAW properties of AlN films were investigated in detail to determine which oriented AlN can support pure shear mode.

Results and Discussion

The three-dimensional acoustic wave equation, in general, is referred to as the Christoffel equation, which can be obtained by substituting constitutive relations into governing equations [14]. It admits three solutions, the properties of which are determined by the relationship of the propagation direction and the stiffness matrix. For materials without piezoelectricity, the Christoffel equation and Christoffel matrix (Γ) take the form

$$k^2\Gamma_{ij}v_j = \rho\omega^2 v_i \tag{1}$$

$$\Gamma_{ij} = l_{iK}c_{KL}l_{Lj}\,, \tag{2}$$

while in a piezoelectric medium the stiffen Christoffel matrix is given by

$$\Gamma'_{ij} = l_{iK}\left(c_{KL} + \frac{[e_{Kl}l_j][l_i e_{iL}]}{l_i\varepsilon^S_{ij}l_j}\right)l_{Lj}\,. \tag{3}$$

In eqs. (1) to (3), v is the particle velocity, l_{iK} or l_i the propagation direction matrix, c the stiffness matrix, ε the permittivity matrix, e the piezoelectric matrix, k the wave number, ω the angular frequency and ρ the density.

The elements in the 3 × 3 Christoffel matrix are functions of material properties of piezoelectric materials and the propagation direction of acoustic waves. The material constants of the AlN are listed in Table I [14]. With the knowledge of AlN material constants and the propagation direction of acoustic wave, the stiffen Christoffel matrix defined in eq. (3) can be solved numerically. Solving the Christoffel matrix gives us three eigenvalues and associated eigenvectors; the eigenvalue is the phase velocity of the acoustic wave and the eigenvector tells us the corresponding vibration direction of the particle (mode).

The piezoelectric coupling constant (K^2) can be obtained using the following equation [14]:

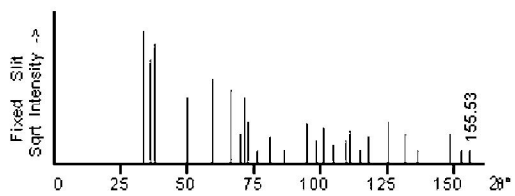
$$v'_a = v_a(1+K^2)^{1/2}, \tag{4}$$

where v'_a and v_a are the stiffened and unstiffened phase velocities, respectively.

Fig. 1 illustrates the Joint Committee on Powder Diffraction Standards (JCPDS) card of AlN (JCPDS 25-1133). The (002)-oriented AlN mean that a preferred orientation of the c-axis is normal to the substrate surface. The (100)-oriented AlN mean that a preferred orientation of the c-axis is parallel to the substrate surface.

Table I Material Constants of AlN.

Density (kg/m^3)	ρ	3512
Elastic stiffness (GPa)	c_{11}	345
	c_{12}	125
	c_{13}	120
	c_{33}	395
	c_{44}	118
	c_{66}	110
Piezoelectric stress constant (C/m^2)	e_{15}	-0.48
	e_{31}	-0.45
	e_{33}	1.55
Dielectric permittivity (ε_0)	ε_{11}	9
	ε_{33}	11



2θ	int-f	h	k	l	2θ	int-f	h	k	l	2θ	int-f	h	k	l
33.216	100	1	0	0	76.445	1	0	0	4	114.83	<1	2	0	4
36.041	60	0	0	2	81.089	4	2	0	2	118.09	4	3	0	0
37.917	80	1	0	1	85.941	1	1	0	4	125.10	10	2	1	3
49.816	25	1	0	2	94.843	9	2	0	3	131.51	5	3	0	2
59.350	40	1	1	0	98.293	3	2	1	0	136.34	1	0	0	6
66.054	30	1	0	3	101.06	7	2	1	1	148.27	5	2	0	5
69.731	5	2	0	0	104.83	2	1	1	4	152.45	1	1	0	6
71.440	25	1	1	2	108.63	3	2	1	2	155.53	<1	2	1	4
72.629	10	2	0	1	111.12	6	1	0	5					

Fig. 1 JCPDS card of AlN.

BAW properties of the (002)-oriented AlN

For an (002)-oriented AlN, the acoustic wave is traveling in the z-direction with $l = \hat{a}_z$ and the corresponding stiffen Christoffel matrix can be derived from eq. (3) as given by

$$\Gamma'_{002} = \begin{bmatrix} c_{44} & 0 & 0 \\ 0 & c_{44} & 0 \\ 0 & 0 & c_{33} + \dfrac{e_{33}^2}{\varepsilon_{33}} \end{bmatrix}. \quad (5)$$

From eq. (5), one can obtain three sets of eigenvalues and associated eigenvectors. They are 1) eigenvalue c_{44} and eigenvector [100], 2) eigenvalue c_{44} and eigenvector [010], and 3) eigenvalue $c_{33} + (e_{33}^2/\varepsilon_{33})$ and eigenvector [001]. Thus, we obtain two pure shear mode and one pure stiffen longitudinal mode with K^2 being equal to $e_{33}^2/c_{33}\varepsilon_{33}$.

Using the material constants of AlN in Table I, one can obtain the pure longitudinal mode with phase velocity 10931 m/s and K^2 6.245 %. While for the two pure shear modes, the phase velocity is 5796 m/s and the K^2 is 0. It is evident that the (002)-oriented AlN can only provide a pure longitudinal mode.

BAW properties of (100)-, (200)- and (300)-oriented AlN

For the (100)-, (200)- and (300)-oriented AlN, the acoustic wave is propagating in the x-direction with $l = \hat{a}_x$. Following the same token, the stiffen Christoffel matrix takes the form

$$\Gamma'_{100} = \Gamma'_{200} = \Gamma'_{300} = \begin{bmatrix} c_{11} & 0 & 0 \\ 0 & c_{66} & 0 \\ 0 & 0 & c_{44} + \dfrac{e_{15}^2}{\varepsilon_{11}} \end{bmatrix}. \quad (6)$$

By solving the Christoffel matrix of the (100)-, (200)- and (300)-oriented AlN, eq. (6), we can obtain one pure longitudinal mode with phase velocity $(c_{11}/\rho)^{1/2}$, one pure shear mode with phase velocity $(c_{66}/\rho)^{1/2}$, and one stiffen shear mode with phase velocity $[(c_{44} + e_{15}^2/\varepsilon_{11})/\rho)^{1/2}$ and K^2 being equal to $e_{15}^2/c_{44}\varepsilon_{11}$. With the material properties given in Table I, the pure longitudinal mode has the phase velocity 9911 m/s, the pure slow shear mode has the phase velocity 5597 m/s, and the stiffen, fast shear mode has the phase velocity 5867 m/s and K^2 2.45 %. Therefore, the (100)-, (200)- and (300)-oriented AlN provided a pure fast shear mode.

BAW properties of (110)-oriented AlN

For an (110)-oriented AlN, the acoustic wave is propagating in the direction with $l = \hat{a}_x(1/\sqrt{2}) + \hat{a}_y(1/\sqrt{2})$. The corresponding stiffen Christoffel matrix of (110)-oriented AlN can be obtained as given by

$$\Gamma'_{110} = \begin{bmatrix} \dfrac{c_{11} + c_{66}}{2} & \dfrac{c_{12} + c_{66}}{2} & 0 \\ \dfrac{c_{12} + c_{66}}{2} & \dfrac{c_{11} + c_{66}}{2} & 0 \\ 0 & 0 & c_{44} + \dfrac{e_{15}^2}{\varepsilon_{11}} \end{bmatrix}. \quad (7)$$

From eq. (7), one can obtain three sets of eigenvalues and associated eigenvectors. They are 1) eigenvalue c_{11} and eigenvector [110], 2) eigenvalue c_{66} and eigenvector [-110], and 3) eigenvalue $c_{44} + (e_{15}^2/\varepsilon_{11})$ and eigenvector [001]. Thus, we obtain one quasi longitudinal, one quasi shear mode, and one pure stiffen shear mode with K^2 being equal to $e_{15}^2/c_{44}\varepsilon_{11}$.

Using the material properties of AlN in Table I, the quasi longitudinal mode has the phase velocity 9911 m/s,

the quasi slow shear mode has the phase velocity 5597 m/s, and the stiffen, pure fast shear mode has the phase velocity 5867 m/s and K^2 2.45 %. Therefore, the (110)-oriented AlN can also provide a pure fast shear mode.

BAW properties of (210)-oriented AlN

For an (210)-oriented AlN, the acoustic wave is propagating in the direction with $l = \hat{a}_x(2/\sqrt{5}) + \hat{a}_y(1/\sqrt{5})$. The corresponding stiffen Christoffel matrix of (210)-oriented AlN can be obtained as given by

$$\Gamma'_{210} = \begin{bmatrix} \frac{4c_{11}+c_{66}}{5} & \frac{2c_{12}+2c_{66}}{5} & 0 \\ \frac{2c_{12}+2c_{66}}{5} & \frac{c_{11}+4c_{66}}{5} & 0 \\ 0 & 0 & c_{44}+\frac{e_{15}^2}{\varepsilon_{11}} \end{bmatrix}. \quad (8)$$

From eq. (8), one can also obtain three sets of eigenvalues and associated eigenvectors. They are 1) eigenvalue A_1 and eigenvector B_1, 2) eigenvalue A_2 and eigenvector B_2, and 3) eigenvalue $c_{44} + (e_{15}^2/\varepsilon_{11})$ and eigenvector [001]. Thus, we also obtain one quasi longitudinal mode, one quasi shear mode, and one pure stiffen shear mode with K^2 being equal to $e_{15}^2/c_{44}\varepsilon_{11}$. The eigenvalues A_1 and A_2 and the associated eigenvectors B_1 and B_2 are defined as follows

$$A_1 = \frac{c_{11}+c_{66}}{2} + \frac{1}{10}\sqrt{9c_{11}^2 + 16c_{12}^2 - 2(9c_{11}-16c_{12})c_{66} + 25c_{66}^2} \quad (9)$$

$$A_2 = \frac{c_{11}+c_{66}}{2} - \frac{1}{10}\sqrt{9c_{11}^2 + 16c_{12}^2 - 2(9c_{11}-16c_{12})c_{66} + 25c_{66}^2} \quad (10)$$

$$B_1 = [\frac{3c_{11} - 3c_{66} + \sqrt{9c_{11}^2 + 16c_{12}^2 - 2(9c_{11}-16c_{12})c_{66} + 25c_{66}^2}}{4(c_{12}+c_{66})}, 1, 0] \quad (11)$$

$$B_2 = [-\frac{-3c_{11} + 3c_{66} + \sqrt{9c_{11}^2 + 16c_{12}^2 - 2(9c_{11}-16c_{12})c_{66} + 25c_{66}^2}}{4(c_{12}+c_{66})}, 1, 0] \quad .(12)$$

Using the material properties of AlN in Table I, the quasi longitudinal mode has the phase velocity 9911 m/s, the quasi slow shear mode has the phase velocity 5597 m/s, and the stiffen, pure fast shear mode has the phase velocity 5867 m/s and K^2 2.45 %. Therefore, the (210)-oriented AlN can also provide a pure fast shear mode.

CONCLUSIONS

The BAW properties of the (100)-, (002)-, (110)-, (200)-, (210)- and (300)-oriented AlN were investigated in this study. It was found that the (002)-oriented AlN can provide a pure longitudinal mode and the (100)-, (110)-, (200)-, (210)- and (300)-oriented AlN can support a pure fast shear mode with the phase velocity 5867 m/s and the K^2 value being 2.45 %.

ACKNOWLEDGEMENT

This research was supported by the National Science Council of Republic of China, under grant no. NSC-95-2221-E-272-001.

REFERENCES

[1] K. M. Lakin, J. S. Wang, G. R. Kline, A. R. Landin, Y. Y. Chen, and J. D. Hunt, "Thin film resonators and filters," *IEEE Ultrasonic Symp.*, pp. 466-475, 1982.

[2] K. M. Lakin, G. R. Kline, R. S. Ketcham, A. R. Landin, W. A. Burkland, K. T. McCarron, S. D. Braymen, and S. G. Burns, "Thin film resonator technology," *IEEE 41st Annu. Symp. Frequency Contro*l, pp. 371-381, 1987.

[3] K. M. Lakin, G. R. Kline, R. S. Ketcham, J. T. Martin, and K. T. McCarron, "Stacked crystal filters implemented with thin films," *IEEE Proc. 43rd Annu. Symp. Frequency Control*, pp. 536-543, 1989.

[4] R. Jakkaraju, G. Henn, C. Shearer, M. Harris, N. Rimmer and P. Rich, "Integrated approach to electrode and AlN depositions for bulk acoustic wave (BAW) devices," *Microelectron. Eng.*, vol. 70, pp. 566-570, 2003.

[5] T. Nishihara, T. Yokoyama, T. Miyashita, and Y. Satoh, "High performance and miniature thin film bulk acoustic wave filters for 5 GHz," *Proc. IEEE Ultrasonic Symp.*, vol. 1, pp. 969-972, 2002.

[6] R. Lanz and P. Muralt, "Bandpass filters for 8 GHz using solidly mounted bulk acoustic wave resonators," *IEEE Trans. Ultrason., Ferroelectr., Freq. Control*, vol. 52, pp. 936-946, 2005.

[7] H. P. Lobl, M. Klee, R. Milsom, R. Dekker, C. Metzmacher, W. Brand, and P. Lok, "Materials for bulk acoustic wave (BAW) resonators and filters," *J. Eur. Ceram. Soc.*, vol. 21, pp. 2633-2640, 2001.

[8] V. Mortet, M. Nesladek, J. M'Dhaen, G. Vanhoyland, O. Elmazria, M. B. Assouar, P. Alnot, and M. B. D'Olieslaeger, "Deposition of aluminium nitride film by magnetron sputtering for diamond-based surface acoustic wave applications," *Phys. Stat. Sol. A*, vol. 193, pp. 482-488, 2002.

[9] H. Zhang and E. S. Kim, "Micromachined Acoustic Resonant Mass Sensor," *J. Microelectromech. Syst.*, vol. 14, pp. 699-706, 2005.

[10] D. S. Ballantine, R. M. White, S. J. Martin, A. J. Ricco, E. T. Zellers, G. C. Frye, and H. Wohltjen, *Acoustic wave sensors: theory, design, and physico-chemical applications*. New York: Academic Press, 1996.

[11] S. M. Reddy, J. P. Jones, and T. J. L. Lewis, "The coexistence of pressure waves in the operation of quartz-crystal shear-wave sensors," *J. Appl. Phys.*, vol. 83, pp. 2524-2532, 1998.

[12 L. McKenna, M. I. Newton, G. McHale, R. Lucklum, and J. Schroeder, "Compressional acoustic wave generation in micro-droplets of water in contact with quartz crystal resonators," *J. Appl. Phys.*, vol. 89, pp. 676-680, 2001.

[13] G. Kovacs and A. Venema, "Theoretical comparison of sensitivities of acoustic shear-wave modes for (bio)chemical sensing in liquids," *Appl. Phys. Lett.*, vol. 61, pp. 639-641, 1992.

[14] J. F. Rosenbaum, *Bulk Acoustic Wave Theory and Devices*. Boston: Artech House, 1998.

[15] J. G. Gualtieri, John A. Kosinski, Arthur Ballato, "Piezoelectric materials for acoustic wave applications," *IEEE Trans. Ultrason., Ferroelectr., Freq. Control*, vol. 41, pp. 53-59, 1994.