VIBRATION ENERGY HARVESTERS BASED ON C-AXIS TILTED ALN THIN FILMS

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Abstract: This study aims to clarify the piezoelectric characteristics of AlN thin films with specific crystallographic direction and to fabricate AlN thin films with specific crystallographic orientation. Theoretical study of dependence of piezoelectric strain and stress coefficients (d_{31} and e_{31}, respectively) and electromechanical coupling factor (k_{31}) as a function of crystallographic direction from the *c*-axis were conducted. AlN thin films were deposited using electron cyclotron resonance (ECR) sputtering with changing angle between surface of the substrates and AlN flux, and evaluated by X-ray diffraction (XRD) measurement. XRD patterns suggested the possibility that crystallographic orientation of the AlN thin films changed due to deposition angle.

Keywords: AlN, energy harvester, crystallographic orientation, electromechanical coupling coefficient

INTRODUCTION

In order to supply power to sensor nodes in wireless sensing systems, energy harvesters scavenging energy from the environment are attractive replacement because of their longer life time and lower maintenance cost [1]. For the energy harvesters, mechanical vibration is one of the attractive power sources, because it has better reliability and higher power density [2] compared to light, radio-frequency (RF), and electromagnetic radiation. In order to convert mechanical energy into electricity, piezoelectric systems have the advantages against electromagnetic and electrostatic ones [3] in seize, energy conversion efficiency, and simpleness of structures. A material often used for energy harvesters fabrication is lead zirconate titanate ($Pb[Zr_xTi_{1-x}]O_3$, PZT). PZT, however, has been considered to be environmentally hazardous due to toxic Pb. Thus recently Pb-free aluminum nitride (AlN) thin films have attracting attention as an alternative to PZT.

As equation (1) indicates, one of the dominating parameters for output power of the energy harvesters is an electromechanical coupling coefficient k_{31} of the piezoelectric materials determining energy conversion efficiency between mechanical and electrical energy.

$$Optimal\ Power \propto k_{31}^2 \cdot m_{eff} \cdot \frac{a^2}{f_r} \cdot Q^2 \tag{1}$$

where k_{31}, m_{eff}, a, f_r and Q are electromechanical coupling coefficient, effective mass, acceleration, resonant frequency and quality factor respectively [4]. To maximize the output power of the energy harvesters, one should adopt the specific crystallographic direction of the piezoelectric materials, along which the k_{31} becomes maximum. In case of the AlN thin film, k_{31} depends on its crystallographic direction in the same way as it changes in a zirconium oxide thin film [5], though usually a single crystal AlN thin film with *c*-axis oriented normal to the substrate is adopted for the energy harvesters [6].

In this study, we theoretically investigated dependence of the k_{31} on the crystallographic direction of the AlN thin films, and experimentally challenged fabrication of the AlN thin films with specific crystallographic direction normal to the substrate.

THEORETICAL

Dielectric permittivity ε', piezoelectric stress coefficient e' and elastic stiffness c' of AlN thin films can be calculated by the following equations using values already known for those of the AlN thin films with *c*-axis normal to the substrate [7].

$$\varepsilon' = a\varepsilon a^t \tag{2}$$
$$e' = aeM^t \tag{3}$$
$$c' = McM^t \tag{4}$$

$$a = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix} \tag{5}$$

$$M=\begin{bmatrix} a_{11}^2 & a_{12}^2 & a_{13}^2 & 2a_{12}a_{13} & 2a_{11}a_{13} & 2a_{11}a_{12} \\ a_{21}^2 & a_{22}^2 & a_{23}^2 & 2a_{22}a_{23} & 2a_{21}a_{23} & 2a_{21}a_{22} \\ a_{31}^2 & a_{32}^2 & a_{33}^2 & 2a_{32}a_{33} & 2a_{31}a_{33} & 2a_{31}a_{32} \\ a_{21}a_{31} & a_{22}a_{32} & a_{23}a_{33} & a_{22}a_{33}+a_{23}a_{32} & a_{21}a_{33}+a_{23}a_{31} & a_{21}a_{32}+a_{22}a_{31} \\ a_{11}a_{31} & a_{12}a_{32} & a_{13}a_{33} & a_{12}a_{33}+a_{13}a_{32} & a_{11}a_{33}+a_{13}a_{31} & a_{11}a_{32}+a_{12}a_{31} \\ a_{11}a_{21} & a_{12}a_{22} & a_{13}a_{23} & a_{12}a_{23}+a_{13}a_{22} & a_{11}a_{23}+a_{13}a_{21} & a_{11}a_{22}+a_{12}a_{21} \end{bmatrix} \quad (6)$$

where θ, ε, e and c is the tilting angle of AlN c-axis to substrate normal, dielectric permittivity, piezoelectric stress coefficient and elastic stiffness of AlN with c-axis normal to substrate. The elastic compliance, s, of tilted AlN thin films is the inverse of the elastic stiffness. Then piezoelectric strain coefficient can be obtained by the simplified equation (7)

$$d_{31}=e_{31}\bullet s_{11} \quad (7)$$

where d_{31}, e_{31}, and s_{11} is piezoelectric strain coefficient, piezoelectric stress coefficient and elastic compliance respectively. Finally, the mechanical electrical coupling factors are calculated by equation (8)

$$k_{31}=(e_{31}^2 s_{11}/\varepsilon_{33})^{1/2} \quad (8)$$

EXPERIMENTAL

An AlN thin film was deposited at 300 ℃ on a Si (100) substrate using electron cyclotron resonance (ECR) sputtering. To fabricate the AlN thin films with specific crystallographic direction normal to the substrate, a tilting jig [8] as indicated in the Fig. 1 was used to hold the substrate. This design allows the particle flux coming from the bottom to impinge the substrate with an inclination angle $\theta_{\text{inc}}=0°, 30°, \text{and } 50°$. The obtained AlN thin films were characterized by X-ray diffraction (XRD) measurement.

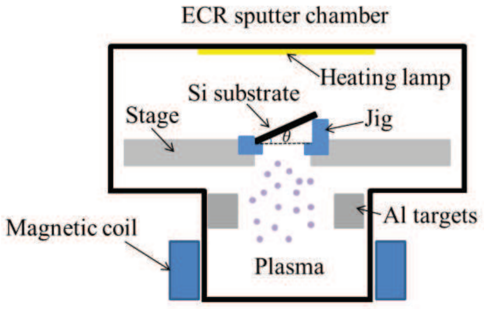
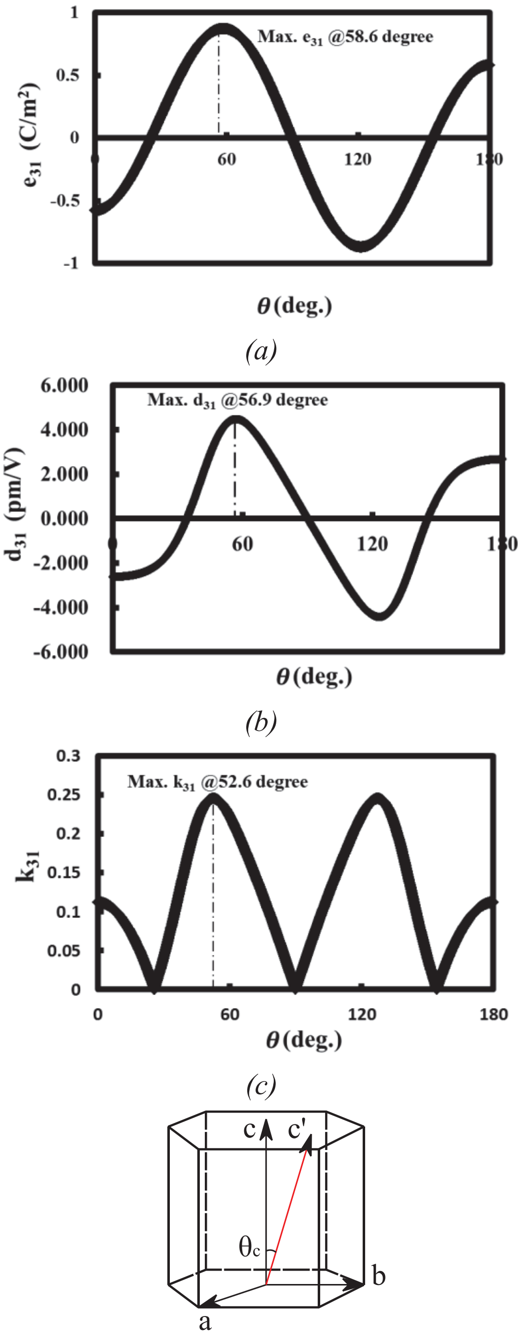


Fig. 1: The schematic of sputtering c-axis tilted AlN

RESULTS AND DISCUSSION

The results of calculation for piezoelectric stress



(a)

(b)

(c)

(d)

Fig. 2:(a) The piezoelectric stress coefficient of tilted AlN thin films, (b) the piezoelectric strain coefficient of tilted AlN thin films, (c) the electromechanical coupling coefficient of tilted AlN thin films, (d) crystallographic direction of tilted AlN unit cell

and strain coefficient (e_{31} and d_{31} respectively), electromechanical coupling coefficient (k_{31}) of the AlN thin films are shown in Figure 2(a)-(c) as a function of crystallographic direction θ_c from the c-axis [see Fig. 2(d)]. Both of the piezoelectric stress coefficient e_{31} [Fig. 2(a)] and the piezoelectric strain coefficient d_{31} [Fig. 2(b)] showed clear dependence on θ_c. The maximum value appeared at $\theta_c = 58.6°$ for d_{31}, and at 56.9° for e_{31}. The value of the k_{31} for different θ_c were calculated by substituting obtained values of the d_{31}, e_{31} and ε_{33} into equation (7) and (8) and plotted in Fig. 2(c). The k_{31} also showed clear dependence on θ_c and showed the maximum at $\theta_c = 52.6°$. The maximum value of 0.244 at $\theta_c = 52.6°$ is 206% as much as that of 0.118 along c-axis at $\theta_c = 0°$.

Figure 3 shows the XRD patterns of the AlN thin films deposited using tilting jigs with $\theta_{\text{inc}} = 0°, 30°, \text{and } 50°$, repspectively. In every patterns, we clearly observed (002) and (004) diffraction peak at $2\theta = 36.0°$ and $76.4°$, respectively. In addition, we observed (100) diffraction peak at $2\theta = 33.2°$, but its intensity was less than two orders of magnitude. This apparently indicated that all the AlN thin films in this study have high degree of c-axis orientation normal to the substrate surface. Closely looking at the (002) diffraction patterns (see the inset), we noticed that peak width became broader and peak position shifted more to the right with increasing the θ_{inc}. The former maybe due to less degree of crystallization or thinner thickness of the AlN thin films with increasing θ_{inc}. The latter may due to change in a distance between nearest neighboring (001) planes.

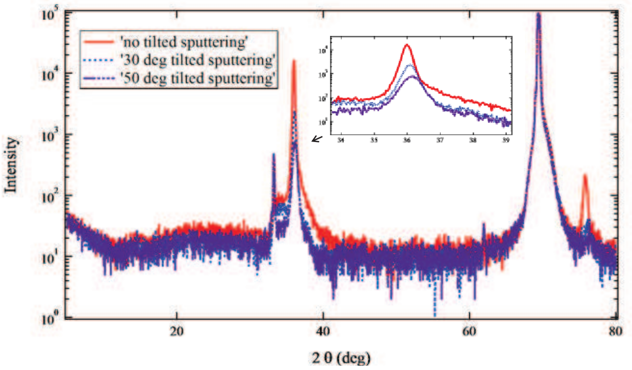


Fig. 3: XRD patterns of AlN thin films deposited using different tilting jigs

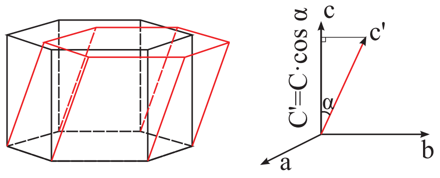


Fig. 4: A unit cell of normal (black) and distorted (red) AlN hexagonal structures

To explain the above mentioned change, we propose one model. Figure 4 shows a unit cell of normal (black) and distorted (red) AlN hexagonal structures. If unit cell of an AlN is distorted in the thin film deposited with $\theta_{\text{inc}} = 30°$ and 50° without changing length of the c-axis, a distance between nearest neighboring (001) planes d_{001} decrease as shown in Fig. 4. If angle between c-axis of normal and distorted AlN unit cell is α, then d_{100} reduces with increasing α as

$$d_{100} = c\cdot\cos\alpha \qquad (9)$$

Figure 5 shows peak angle of the (002) diffraction of the AlN thin films on the left axis as a function of θ_{inc}. The figure indicated that the peak angle shifted almost linearly to the higher angle with increasing θ_{inc}. On the right axis, normalized d_{100} obtained using the values of the peak angle and Bragg's condition was also plotted. The values of d_{100} were used to calculate the angle α between c-axis of normal and distorted AlN unit cells from equation (9).

Figure 6 shows the angle α as a function of θ_{inc}. Provided the previous model of distorted AlN unit cell is the case, the figure indicated that

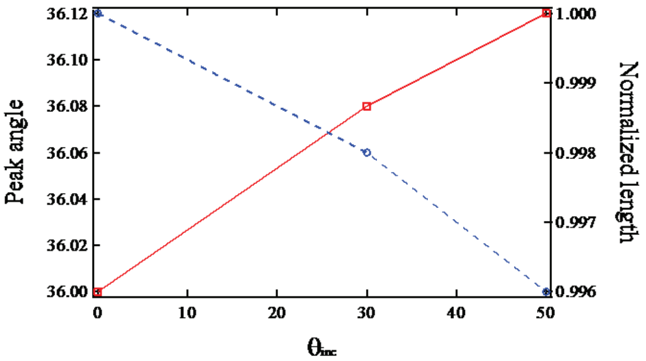


Fig. 5: Peak angles of AlN (002) diffraction (red line) and normalized d $_{100}$ length (blue, dotted line) versus tilting angles of sputtering jig

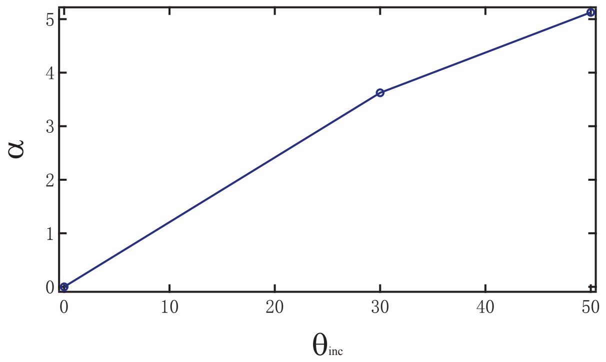


Fig. 6: Calculated distorted angles versus tilting angles of sputtering jig

the α increased almost linearly with increasing θ_{inc}. Further investigation is in progress to verify the unit cell distortion.

CONCLUSION

In this study, dependence of piezoelectric coefficients (d_{31} and e_{31}) and electromechanical coupling factor (k_{31}) on crystallographic direction of AlN thin films are investigated theoretically. AlN thin films with specific crystallographic direction normal to the substrate were fabricated in electron cyclotron resonance (ECR) sputtering with $0°, 30°,$ and $50°$ tilting jigs. The deposited thin films were evaluated by X-ray diffraction (XRD) measurement. The XRD patterns showed high degree of *c*-axis orientation normal to substrate surface. At the same time, a clear shift of peak position of (002) diffraction patterns can be observed. This phenomenon was explained as the change of distance d_{100} between neighboring (001) planes which due to the distortion of AlN unit cell.

ACKNOWLEDGEMENT

The research was supported by NEDO (New Energy and Industrial Technology Development Organization, No. J100002626).

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