## Abstract Submitted for the MAR17 Meeting of The American Physical Society

First-principle studies on the influence of anisotropic pressures on the physical properties of AlN ZHIFAN WANG, Chengdu Green Energy and Green Manufacturing Technology RD Center, YANNING ZHANG, University of Electronic Science and Technology of China, UNIVERSITY OF ELECTRONIC SCIENCE AND TECHNOLOGY OF CHINA COLLABORATION, CHENGDU GREEN ENERGY AND GREEN MANUFACTURING TECHNOLOGY RD CEN-TER COLLABORATION — AlN has been widely used in electro-acoustic mechanical sensors. The performance of those AlN based sensors are usually dominated by its intrinsic physical and electronic properties. In this work, we first performed extensive first-principle studies to discuss the effect of uniaxial and biaxial mechanical pressures on the structural and physical properties of AlN piezoelectric material, including the longitudinal elastic constant  $(C_{33})$ , piezoelectric constant  $(e_{33})$ , static dielectric constant ( $\varepsilon_{33}$ ), and mass density ( $\rho$ ). We give the relationship between the paramters mentioned above and the longitudinal acoustic wave velocity (V) under anisotropic pressures. Our results show that the applied uniaxial or biaxial pressure in the basal plane has a more obvious influence on physical properties of AlN than the uniaxial pressure along hexagonal axis. The pressure-induced variations of  $C_{33}$ ,  $e_{33}$  and  $\rho$  significantly change the V value, whereas that of  $\varepsilon_{33}$  on V is negligible. Our theoretical results provide useful information for the performance predictions of AlN based FBAR mechanical sensors<sup>1</sup> 1. E. Anders, I. Katardjiev and V. Yantchev, J. Micromech. Microeng. 21, 85010-85016(85017) (2011).

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