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Simulation of Longitudinal Mode of Vibration in Piezoelectric Monolayer MoS_2

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Abstract

Monolayer molybdenum disulphide (MoS_2) is one of the desired materials for the new age piezoelectric devices. The main objective of the paper is to present the finite element (FE) simulation of piezoelectric monolayer MoS_2 in COMSOL Multiphysics software. A rectangular MoS_2 sheet is simulated in fixed-fixed end and free-free end configuration. The eigenmode analysis is done and the eigen frequency is calculated. Due to the presence of one molecular layer and piezoelectric matrix the vibration should be in longitudinal mode. The longitudinal acoustic velocity is also calculated from the simulation and is verified analytically.

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Keywords: MoS_2 sheet; monolayer; NEMS; FE simulation

1. Introduction

From the time of its discovery, piezoelectricity is one of the most applied theories in the development of actuators and sensors [1]. With the emergence of microelectromechanical systems (MEMS) and nanoelectromechanical systems (NEMS), demand for suitable piezoelectric materials was felt. It motivated new theoretical and experimental research on piezoelectric materials in nanometer range like nanotubes, nanowires and single molecules [2-4]. After the discovery of graphene, the development of nanostructures of single molecular layer became the new path of research in the area of nanotechnology. Mainly the absence of bandgap in graphene prompted the development of

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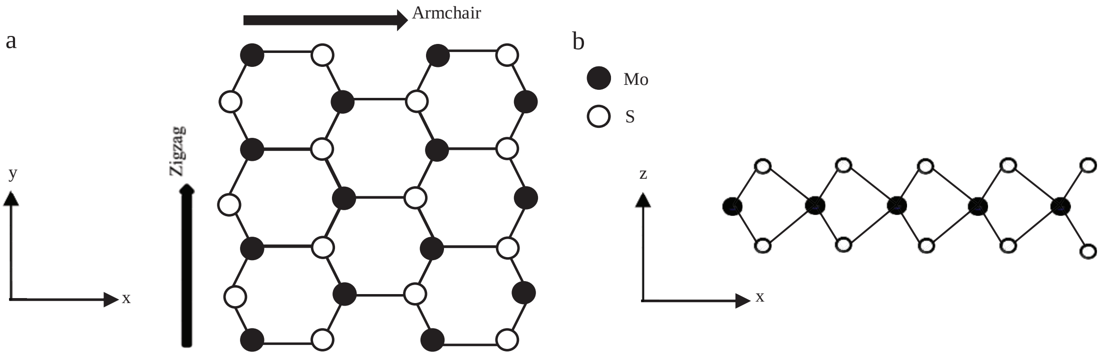

Fig. 1. (a) Top view of hexagonal crystal structure of MoS_2 showing two different edge configurations; (b) Side view of MoS_2 monolayer showing lack of inversion center.

monolayer molybdenum disulfide (MoS_2) as a new two-dimensional semiconductor having direct bandgap property. MoS_2 for the last couple of years has been reported as a promising candidate in low dimensional electronics [5]. Due to its excellent mechanical properties like high in-plane stiffness and ability of withstanding large strains, monolayer MoS_2 has applications in MEMS and NEMS fields. It has been reported in the development of sensors [6], resonators [7], and dc contact switches [8].

MoS_2 belongs to the family of transition metal dichalcogenide (TMDC) with other materials like BN, $MoSe_2$, $MoTe_2$, and WS_2. These TMDC materials are centrosymmetric in bulk form shown in Fig. 1(a) but in monolayer form they become noncentrosymmetric because of the absence of inversion center. Theoretically it has been predicted earlier [9] that TMDC materials will exhibit piezoelectricity in monolayer form of having no inversion center as shown in Fig. 1(b). Thus these monolayer materials including MoS_2 show possible applications in the field of two dimensional piezoelectric materials. It is found that monolayer MoS_2 has piezoelectric coefficient d_{11} = 3.73 pm/V which is greater than GaN (d_{33} = 3.1 pm/V) [9]. Fig. 2 represents the comparison of the piezoelectric coefficients of monolayer MoS_2 and different piezoelectric bulk materials. Though some bulk materials have greater piezoelectricity than MoS_2, the single layer MoS_2 has unique advantages of lightweight, high stiffness, and high surface to volume ratio. Therefore greater sensitivity and compact size can be realized when MoS_2 monolayer is used as a piezoelectric device.

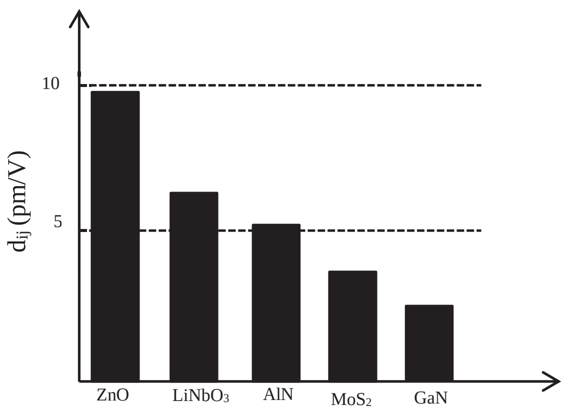

Fig. 2. Comparison between piezoelectric coefficients of monolayer MoS_2 and different piezoelectric bulk materials [9].