Available online at www.sciencedirect.com

ScienceDirect

Procedia IUTAM 21 (2017) 56 – 62

Procedia IUTAM

www.elsevier.com/locate/procedia

2016 IUTAM Symposium on Nanoscale Physical Mechanics

Influence of Flexoelectric effects on current-voltage characteristic of polydomain in ferroelectric thin films

Limei Jiang[a,b*], Xiaofei Xu[a] ,Yichun Zhou[a,b†]

[a]*Hunan Provincial Key laboratory of Thin Film Materials and Devices, School of Materials Science and Engineering, Xiangtan University, Xiangtan 411105, Hunan, China*

[b]*Key Laboratory of Key Film Materials & Application for Equipment of Hunan province, Xiangtan University, Xiangtan 411105, Hunan, China*

Abstract

Strain gradients at domain walls in polydomain ferroelectric thin films generally are huge, reaching a value of 10^7-10^8 m^{-1}, appears at domain walls. These huge strain gradients always play a considerable impact on polarization distribution via flexoelectricity. However, the ability of the flexoelectricity to tune the leakage current in ferroelectric nanofilms is untouched to date. By combining the phase field model and diffusion equations for an electron/electron hole, a self-consistent model is established to investigate the influence of flexoelectric effect on the current-voltage characteristic of Pt/Pb($Zr_{0.1}Ti_{0.9}$)O_3/Pt capacitor. It is shown that the longitudinal flexoelectric coefficient related coupling type would reduce the electric potential, and thus, increase the electron hole concentration and cause leakage current increasing in thin films. In contrast, the transverse flexoelectric coefficient related coupling type would raise the electric potential, decrease the electron hole concentration and cause leakage current decreasing in thin films.

Peer-review under responsibility of organizing committee of Institute of the 2016 IUTAM Symposium on Nanoscale Physical Mechanics

Keywords: Flexoelectric effect; Dislocation; Domain; Phase field method;

1. Introduction

Thanks to their excellent properties such as ferroelectricit[1-5], dielectricity[6], piezoelectricity[7], pyroelectricity[8]

* Corresponding author. Tel.: 0731-58293586
Email address: lmjiang@xtu.edu.cn

† Corresponding author. Tel.: 0731-58293586
Email address: zhouyc@xtu.edu.cn

Peer-review under responsibility of organizing committee of Institute of the 2016 IUTAM Symposium on Nanoscale Physical Mechanics
doi:10.1016/j.piutam.2017.03.037

optical nonlinearity[9] etc., ferroelectric thin films have attracted a great deal of attention and are one of the most promising technology in advanced memories[10,11], integrated optics[12] and so on. Though as promising as the ferroelectric thin films are, there are still obstacles to be overcome before thin films broad applications. At present, even high quality ferroelectric thin films possess some undesirable properties, leakage current for instance.[13] The leakage current problem plays an especially prominent role in hindering development of the ferroelectric thin films.[14] It has been proved that the leakage current in ferroelectric thin films is closely linked with spatial carriers transport.[15] Thus investigating the carriers transport behaviors in ferroelectric thin films is an essential step in the development of ferroelectric thin films.Previous studies demonstrate that transport behaviors of various ferroelectric devices, for example the electronic conductor-insulator transition[16], the capacitance-voltage characteristics of metal-ferroelectric-metal structures[17] and unidirectional electron conduction[18] can be readily achieved by controlling the polarization. Therefore, methods that could effectively control polarization in ferroelectrics are indispensable for us to obtain the desirable transport behaviors. For nanoscale epitaxial ferroelectric thin films, in which the strain gradient can be relaxed within tens of nanometers, the resulting flexoelectric field can become as large as 10 MVm^{-1}.[19] There is a growing body of evidences indicating that flexoelectricity[20-24] can provide routes of tuning polarization behaviors in nano ferroelectrics. Theoretically, Catalan[25], Jiang et al.[21] observed that the strain gradient can change domain structures and polarization switching behaviors. On the other hand, recent experimental studies on flexoelectricity-driven phenomena demonstrated that strain gradient can induce a rectifying transport bahavior[19], poling[26], switching[21,22,27] and rotation of polarization.[28] Here, it is important to notice that Lee[19] and Lu[27] et al. observed that strain gradient generated by the misfit strain in single crystal film of $HoMnO_3$ or the tip force of an atomic force microscope on polycrystalline $HoMnO_3$ thin film can rectify the carriers transport behavior of $HoMnO_3$ via flexoelectricity. It is found that by affecting the distributions and transport of the charged carries in ferroelectric thin films, the flexoelectric field induced by the strain gradient plays a pivotal role eventually changing the transport behaviors.[19]

Even though this experimental report results are remarkable and conspicuous, our understanding of the underlying mechanism is still rather limited and deficient. For example, in usual, a ferroelectric thin film is composed of complex polydomain configuration. No reports, however, have shown whether the transport behaviors in polydomain would be affected by flexoelectric effect. Besides, for a material belongs to cubic point group, there are three independent components of the flexoelectric coefficients: f_{1111}, f_{1122} and f_{1212}[29]. What role each flexoelectric tensor component plays in the transport behavior of ferroelectric thin films? Thus, to complement the experimental studies and fully understand the transport behaviors, theoretical models and computational simulations that can describe the coupling between ferroelectric polarization and charged carriers transport are of great demand.

The motivation of this study is to develop a self-consistent model to understand the influence of flexoelectric effect on transport behavior of polydomain ferroelectric thin film. This model is developed combining the phase field method of flexoelectricity[30], Mindlin's strain gradient theory[21] and diffusion equations for electron/hole transport[31]. Finite element method is used to solve the model equations.

We are interested in determining what role each flexoelectric tensor component plays in the transport behaviors of $Pb(Zr_{0.1}Ti_{0.9})O_3$ (PZT) ferroelectric thin films. For this purpose, we took two cases into consideration: (a) $f_{11}^* \neq 0$, $f_{12}^*=0$, $f_{44}^*=0$; (b) $f_{11}^*=0$, $f_{12}^* \neq 0$, $f_{44}^*=0$, where f_{11}^*, f_{12}^* and f_{44}^* are the Voigt forms of the flexoelectric tensors f_{1111}, f_{1122} and f_{1212}, respectively. As for f_{44}^*, which describes the coupling between shear strain gradient and polarization, it was neglected since the shear strain gradient is one order smaller than the normal strain gradients in ferroelectric thin films.[22] It was found that flexocoupling would influence the transport behaviors of PZT ferroelectric thin film. Different flexocoupling types, i.e., the longitudinal and transverse flexoelectric coefficient related coupling types have distinct impacts on the leakage current in ferroelectric thin films. The longitudinal flexoelectric coefficient related coupling type strengthens the conduction of PZT thin film, in other words, increases the leakage current. This phenomenon, however, became completely different for the transverse flexoelectric coefficient related coupling type.

2. Phase field method