CHAPTER 1

Introduction

1.1 Overview

Ferroelectric materials are one of vital components widely used in many electronic devices such as dynamic random access memories (DRAMs), non-volatile ferroelectric random access memories (FRAMs), infrared sensors, capacitors, and actuators [1-3], because they have interesting electronic and optical properties. Moreover, they can be grown as thin films, which allow them to be applied in modern circuits [4]. These interesting properties include extremely low coercivity, high remnant polarization, polarization switching [5], better mechanical strength, small deviation in composition, high dielectric constant, pyroelectricity—the ability of certain materials to produce an electric potential when they are heated or cooled, piezoelectricity—the ability of certain materials to generate an electric current when they are subjected to mechanical stress, and photorefractive effect—the ability of certain materials to response to light when they are changed their refractive index [6].

An essential feature of ferroelectric materials is the spontaneous polarization that can be reversed by the application of an electric field. Consequently, they can exhibit polarization-electric field hysteresis loops similar to ferromagnetic materials. This means that ferroelectric materials exist tiny regions called ferroelectric domains. The presence of an external electric field with altering intensity makes ferroelectric domains changes size and shape. To deeply understand physical behaviors, ferroelectric materials are investigated through their hysteresis loops under many external perturbations [7-12]. Ferroelectric hysteresis loops can be simulated by various theoretical models such as the mean-field based on the Ising model [13-15] and Heisenberg model [16], and Monte Carlo method based on spin models [17, 18]. After simulating, ferroelectric properties can be extracted from ferroelectric hysteresis loops. A dynamic hysteresis loop has now been considered important in both fundamental and technological point of view in terms of their associates, such as hysteresis shape, hysteresis loop area, remnant polarization, coercive electric field. For instance, the hysteresis loop area is the energy dissipated within one cycle of dipole switching, which identifies the nature of phase transition between ferro- and para-phase. Moreover, the remnant polarization and coercive field show the stability of the ordered alignment at nonzero temperature.

The studies in such a topic become interesting subject from the point of view of application, due to the high-speed memory devices in which ferroelectric thin films are being developed extensively. The responses of ferroelectric thin films to external fields including the structure of thin films, such as thin film's thickness, were investigated in detail to design better devices [19]. Moreover, The responses of ferroelectric materials under many different conditions, for example, the combination of periodic electric field and static stress field [20], static electric field and periodic stress field [21], or periodic electric and stress fields [22], were intensively investigated.

Although many ferroelectric systems under various conditions had been studied and reported, physical properties of ferroelectric thin films affected by these external perturbations have not been quite well recognized, due to the complexity of thin film's thickness. Therefore, a more realistic model which includes the effects of structural defects, such as partial non-polarizable structure, should be considered, in detail. In this thesis, the Monte Carlo simulation was employed to investigate the properties of various ferroelectric systems with partial non-polarizable structure under external perturbations. This study is not directly focused on applications of ferroelectric materials, but the obtained results should be useful for the understanding and improvement of ferroelectric devices.

1.2 Research objectives

The main objectives of this research work are to study ferroelectric materials with partial non-polarizable structure and to find out how this imperfect structure influences ferroelectric materials under external perturbations such an external electric field, a stress field, or a combination of external electric and stress fields.

1.3 Scope of study

This research work focuses on ferroelectric materials with partial non-polarizable structure under external perturbations. We focus on the following situations:

(1) Dynamic hysteresis properties of ferroelectric thin films with varying thickness under an external electric field.

(2) Phase transitions in ferroelectric thin films under an external electric field.

(3) Hysteresis behaviors of ferroelectric ultra-thin films under external electric and stress fields.

In this thesis, spin models including DIFFOUR model, Heisenberg model with DIFFOUR type interaction, and 2D four-state Pott model are considered. Physical properties of ferroelectric systems are studied through their hysteresis loops simulated by Monte Carlo method. Metropolis algorithm, free or/and periodic boundary condition are taken into account.

1.4 Thesis outline

We organize this thesis into five chapters as following:

Chapter 1 introduces the general information about studying properties and applications of ferroelectric materials, research objectives, and scope of this study.

Chapter 2 says the research works about ferroelectric materials in details, ferroelectric hysteresis area, fundamental analysis and data analysis used to study ferroelectric hysteresis behaviors under various external perturbations. Fundamental analysis includes spin models, mean-field theory and Monte Carlo method. Data analyzing consists of artificial neural network and Fourier transformation.

Next, the Hamiltonians for ferroelectric materials with partial non-polarizable structure are proposed in Chapter 3. This chapter shows also how to assign non-polarizable sites on a unit cell as well as how to extract some results from a single simulation at a given temperature. We can obtain one function at one temperature from a simulation at another temperature.

Later, Chapter 4 consisting of the results and discussions shows the roles of ferroelectric materials with partial non-polarizable structure on hysteresis behaviors under an external electric field, and a combination of external electric and stress fields. These external fields are considered as time-dependent functions to investigate the change in directions of electric polarization.

Finally, Chapter 5 contains the overall conclusions of this study as well as future works that should be proposed.