# CHAPTER 5

## Conclusions and Future Works

### 5.1 Conclusions

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 applied external fields such as an electric field, a stress field, or a combination of external electric and stress fields. Our studies are based on the discrete vector models including the DIFFOUR model, modified Heisenberg model with DIFFOUR type interaction, and 2D four-state Potts model. We choose the Metropolis algorithm to update our system and simulate the ferroelectric hysteresis loops under external perturbations, such as external electric and stress fields, using Monte Carlo method.

We started with assigning the Hamiltonians for the DIFFOUR model, modified Heisenberg model with DIFFOUR type interaction, and 2D four-state Potts model. These considered models were used to simulate ferroelectric materials with partial non-polarizable structure. In preparing our models, we assumed that each ferroelectric dipole is in a unit cell. Each non-polarizable site was placed on one of four sides of a unit cell. Moreover, we investigated the effects of non-polarizable structure on ferroelectric hysteresis behaviors through a parameter called defect concentration $c$.

In during simulating, we updated our ferroelectric systems using Metropolis algorithm. Later, we measured the electric polarization $P$ to create a ferroelectric hysteresis loop, and extracted hysteresis area $A$ from an obtained hysteresis loop. The evolution of hysteresis loops was simulated to investigate hysteresis behaviors of ferroelectric thin films with partial non-polarizable structure. We can conclude that the hysteresis area $A$ depends on many parameters such as field frequencies $f$, field amplitudes $E_0$, thickness of thin films (layers) $l$, defect concentration $c$ and stress field as the following details:

(1) At high frequency region ($f > 0.100$ mcs$^{-1}$), the hysteresis area $A$ decreases with increasing field frequency $f$ because our ferroelectric systems have less time to switch the dipoles of system. Consequently, our systems take less energy to change the direction of dipoles. These results may be useful for designing memory devices because some circumstances with high field frequency may effect on the ability to store data of ferroelectric memory devices.

(2) The hysteresis area $A$ decreases with increasing defect concentration $c$ since the absence of some dipoles may reduce ferroelectric interaction. Consequently, the energy dissipation associated to dipole switching also decreases. These results may be useful for any decisions to choose suitable methods for preparing materials because, during preparing, many electric devices with imperfect structures can occur. Moreover, the dynamic phase transition temperature (from dynamic ferroelectric phase to dynamic paraelectric phase) decreases with increasing defect concentration due to weaker ferroelectric interaction.

(3) With or without defect concentration $c$, the hysteresis area $A$ decrease with increasing the thickness of thin films since there are the stronger ferroelectric interactions. Consequently, our ferroelectric system take more energy to switch the dipoles. These results may be useful to determine appropriately the number of layer of thin films.

(4) Under a free, longitudinal tensile, longitudinal compressive and periodic stress fields, both the coercive field and remnant longitudinal polarization decreases with increasing defect concentration because the dipoles switching into the $z$-direction are inhibited from increasing of defect concentration. These results may be useful for designing ferroelectric devices with non-polarizable structure that is workable under suitable stress field.

(5) The remnant strain decreases with increasing defect concentration under a free or stress fields since most dipoles forced to align along the $z$-direction decrease. These results may be useful for piezoelectric applications such as sensors and actuators as they can efficiently convert mechanical energy into electrical energy and vice versa.

## 5.2 Future Works

There are several observations from this study that have not been explained clearly. It is interesting to further study as following suggestions:

(1) The interaction or coupling terms ($U$, $H_{V1}$, $H_{V2}$, $J$, or $\alpha$) proposed in this thesis should be applied to real materials or experiments.

(2) The effect of stress fields in the $x$-direction on ferroelectric materials with partial non-polarizable structure should be investigated.

(3) The 3D structure or bulk structure should be considered.

(4) The limit of defect concentration for real materials should be further studied.