CHAPTER 5

CONCLUSION

5.1 Conclusion

In this thesis, the local structure distortions of Mn-doped $Bi_{3.25}La_{0.75}Ti_3O_{12}$ (BLT) ceramics and Mn-doped $((K_{0.5}Na_{0.5})_{0.935}Li_{0.065})NbO_3$ (KNNL) ceramics were investigated using x-ray absorption spectroscopy analysis. For Mn-doped BLT, the results show Mn^{4+} substituting on Ti^{4+} octahedral site with the redial distances between Mn^{4+} and O^{2-} in *ab*-axis is almost the same and decreases with increasing Mn-doping contents. This is strong evidence that Mn-doping in BLT can reduce the orthorhombicity, which increases the polarization domains size, enhances remnant polarization, speeds up the polarization domains movement and lessens coercive field. For Mn-doped KNNL, the results show Mn^{3+} substituting on Nb^{5+} octahedral site. The oxygen vacancies in the longest redial distance between Mn^{3+} and O^{2-} in *c*-axis are produced and the remaining redial distances between Mn^{3+} and O^{2-} are more almost the same. This is strong evidence that Mn-doping in KNNL can diminish remnant polarization and increase coercive field. The fundamental understanding of the doping atom role on altering structure and electrical properties can be used as a guideline of how to improve the preparation method to obtain the most efficient electronic devices.

Additionally, the local structure configuration and the formation behavior of lead zinc niobate (PZN) ceramic were investigated by employing a combination of the experimental x-ray absorption spectroscopy analysis and the theoretical first-principles electronic structure calculation. The results show the formation of PZN in pyrochlore phase with Zn^{2+} substituting on Nb^{5+} site with bond length between Zn^{2+} and Pb^{2+} longer than that of perovskite phase. From the different radial distributions of neighboring atoms around Zn^{2+}, the formation energy of the perovskite phase was noticeably found to be higher than that of the pyrochlore phase. This indicates that the steric hindrance of Pb^{2+} lone pair and the mutual interactions between Pb^{2+} lone pair and Zn^{2+} are the main causes of the perovskite phase instability in the lead zinc niobate

material. The fundamental understanding of the formation energy and structural distortion relationship can be used alongside with appropriate synthesis techniques as a guideline to prepare perovskite lead zinc niobate ceramics with exceptional electrical properties.

5.2 Suggestions and future work

The first-principles electronic structure calculation should be performed to support the x-ray absorption spectrum analysis results to obtain better accuracy and reliability level. For instance, the model structure should be relaxed due to the absorbing atom substitution, before calculated x-ray absorption spectra using program FEFF.

Additionally, many important oxide materials require the x-ray absorption spectrum analysis to enhance the fundamental understanding between their structure and their physical properties. For instance, alexandrite is one of the most interesting mineral in laser application that is widely used for medical purposes, as it presents greater performance compared with other lasers. Although, its utilization has been vastly expanded, the location of transition metal impurities mostly iron that is responsible for its special optical properties is not completely understood. The full understanding and control of these optical properties necessitates knowing the precise localization of the transition metal inside the structure. The qualitative XANES analysis could be used to determine site occupation of the Fe^{3+} in the structure of alexandrite ($BeAl_2O_4$) crystal. The accurate site distribution of Fe^{3+} will be useful for doping process to improve the efficiently of alexandrite as a solid-state laser material.