Report on Visit to University of California, Los Angeles by International Training Program

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This report decsripe my research in Professor Jane P. Chang's lab of University of California, Los Angeles (UCLA). The research theme is first principle caculation for magnetoelectrics material (mainly focused on multi-ferrorite), which synthesised by plasma assisted atomic layer deposition (ALD).

A. Introduction of institute

UCLA is a public research university located in the Westwood neighborhood of Los Angeles, California, USA. It was founded in 1919 as the "Southern Branch" of the University of California and is the second oldest of the ten campuses. UCLA, considered as one of the flagship institutions of the University of California system, offers over 300 undergraduate and graduate degree programs in a wide range of disciplines and enrolls about 26,000 undergraduate and about 11,000 graduate students from the United States and around the world. Strengths in liberal arts, sciences and research earned it membership in the association of American Universities [1]. Figure 1 is a picture of Royce hall, one of the landmarks of UCLA.

Fig. 1 Royce Hall, one of the landmarks of UCLA.

The research group in UCLA named "Electronic Materials Synthesis and Plasma Processing Lab" which lead by Professor Jane P. Chang, is mainly focused on the synthesis and patterning of multi-functional complex oxide films with tailored electronic, chemical, thermal, mechanical, and biological properties. Experimental and theoretical studies are combined to understand the process chemistry and surface kinetics in atomic layer deposition, plasma etching and deposition processes, and gas-phase surface functionalization processes. Novel devices including advanced microelectronics, optoelectronics, and chemical sensors are realized at nano-dimensions as the technologies become more enabling based on these fundamental studies [2]. Fig. 2 is author having a lunch with Prof. Chang and her students at faculty center of UCLA.

Fig. 2 The author (seconde from left) having a lunch with Prof. Chang (center) and her students.

B. Research background

Materials that combine magnetic and ferroelectric properties have generated increasing interest over the last few years, due to both their diverse properties and their potential utility in new types of magnetoelectric device application. Here, the basic knowledges concerning the above fields will be introduced.

<u>Magnetoelectric effect</u>

The linear magnetoelectric (ME) effect—induction of magnetization by an electric field or of polarization by a magnetic field is applicable for (i) modulation of amplitudes, polarizations and phases of optical waves, (ii) ME data storage and switching, (iii) optical diodes, (iv) spin-wave generation, (v)

amplification and (vi) frequency conversion were discussed [3]. However, use of the ME effect as a tool in basic research was considered far more promising than engineering applications at that time. Because of its time-asymmetric nature, the ME effect was regarded as a complementary tool for neutron diffraction in the determination of magnetic symmetries and phase transitions and for the observation of antiferromagnetic domains and their manipulation [4].

Multiferroics

Since the ME coupling coefficient in single-phase compounds is small. The only way of achieving a noticeable enhancement of the ME response is to make use of strong internal electromagnetic fields by finding components with a large dielectric or magnetic susceptibility [3]. The largest dielectric coefficients are found in ferroelectrics, while ferromagnets display the largest magnetic permeabilities. Consequently, ferromagnetic ferroelectrics are prime candidates for displaying giant ME effects.

The multiferroics which consisted by two or more of the primary ferroic properties, are united in the same phase are promising systems for ME phase control [5]. In spite of the potential of multiferroics for giant ME effects and ME phase control, the ME effect in multiply ordered singlephase compounds is much farther from practical applications than the ME effect in composite materials. An important step for increasing the flexibility and the number of degrees of freedom in tuning the ME properties of multiferroics is the growth of thin multiferroic films. Thin films are mouldable, and from a compositional point of view typical defects, gradients and deficiencies occurring during bulk growth can be avoided. Chemical substitution is facilitated, and lattice strain, film thickness and an increased range of substituents represent new degrees of freedom for steering the ME properties towards an improved suitability for device applications [3].

Plasma enhanced atomic layer deposition (PEALD)

In order to synthesis these multiferroic thin films, PEALD is proposed as an idea deposition technique that is based on the sequential use of a gas phase chemical process. The majority of PEALD reactions use plasma source and two or more chemicals, typically called precursors. These precursors and plasma react with a surface one-at-a-time in a sequential manner. By exposing the precursors to the growth surface repeatedly, a thin film is deposited [6]. Using PEALD, film thickness depends only on the number of reaction cycles, which makes the thickness control accurate and simple. Moreover, PEALD are the wide range of film materials available, high density and low impurity level. Also, lower deposition temperature can be used in order not to affect sensitive substrates These advantages make the PEALD method attractive for microelectronics for manufacturing of future generation integrated circuits [7].

C. Objective

According to the mechanism underlying multiferroic materials's ferroelectricity is often unconventional [8, 9] as well as the effect of epitaxial strain, defects, microstructure, or interface properties can alter the physical properties of a material, it is nessersary to use first principles calculations to determine intrinsic material properties and explain contradictory experimental data. In this study, the $BiFeO_3$ is used as the prototype material for first principles study.

D. First principle calculation based on density function therory

First principle calculation is an effective way of predicting the material and electronic properties of materials.

Principle of Dnesity functional theory (DFT)

DFT has attained much attention in predicting the atomic level properties of a wide range of materials recently, primarily due to the rapid increase in computational power. With this theory, the properties of a many-electron system can be determined by using functionals, i.e. functions of another function, which in this case is the spatially dependentt on the electron density [10].

Cambridge Serial Total Energy Package (CASTEP)

For caculation, a quantum mechanical program, Cambridge Serial Total Energy Package (CASTEP) was used. CASTEP makes use of the plane-wave pseudopotential total energy calculations within the framework of density functional theory. CASTEP uses state-of-the-art optimization methods to optimize the geometry of a particular structure and the resulting geometry is used to calculate the total energy, electronic band structures, and density of states. The exchange-correlation energy can be chosen from either local-density approximation (LDA) or generalized gradient approximation (GGA). The electronic minimization can be performed using a variety of schemes including the most popular density

mixing scheme [11]. The simple work flow of caculation use CASTEP is shown as Fig. 3.

Fig. 3 Work flow of the calculations.

Bulk electronic structure of $BiFeO_3$

The primitive unit cell of $BiFeO_3$ is shown as Fig. 4. The structure of $BiFeO_3$ can be understood as highly distorted perovskite with rhombohedral symmetry and spece group R3c and relaxed structure has a bond length of 5.6343 Å and rhomobohedral angle 59.348° [12]. After the geometry optimization, the lattice parameters compared with the reported experiment results, showing agreement as summarized in Table 1.

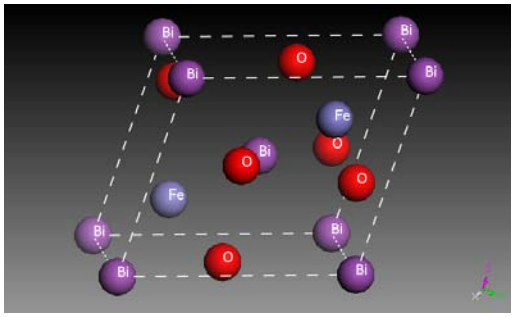

Fig. 4 Structure of R3c $BiFeO_3$.

Table 1 Lattice parameters of $BiFeO_3$.

Lattice Constants	
This work	Reference [13]
a = 5.50 Å	a = 5.35 Å
b = 5.50 Å	b = 5.35 Å
c = 5.50 Å	c = 5.35 Å
α = 59.99°	α = 61.93 °
β = 59.99 °	β = 61.93 °
γ = 59.99 °	γ = 61.93 °

Electrical properties

The electronic structure of $BiFeO_3$ was computed in the ferroelectric *R*3*c* structure. In this study, the single-particle density of states (DOS) for a single spin channel calculated within the LDA as shown in Figs. 5 (a). For BiFeO3 in the *R*3*c* structure, both spin channels exhibit identical total DOSs. The structure is conductor, without gap in the LDA calculation. Previous study shown the insulating properties with a small gap of 0.4 eV as shown in Fig.5 (b) [13]. The contradiction between of these results might be caused by structure optimizing. The further investigation was needed.

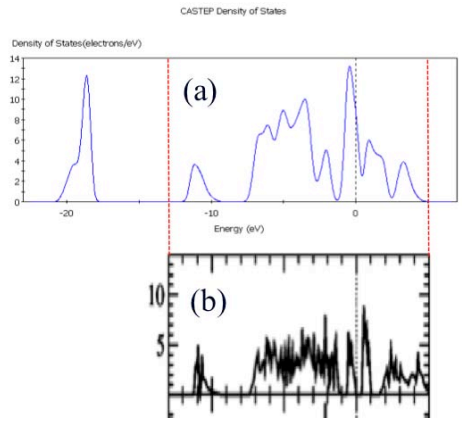

Fig. 5 (a) Calculated densities of states (DOSs) for *R*3*c* BiFeO3. the total DOS for one spin channel calculated within the LDA. (b) reference calculationg result [13].

However, from this study, we can see the potential of first principle caculation, which can help us realize the electrical properties (i.e. polarization) along a path from the structure, and how the defect or impurity affect such properties.

E. Summary

The most important thing during this 2 months in Prof. Chang's group is that I made a lot of friends. I enjoyed very much with the group members, even simply looking at them is also edify me. I learn more than knowledge from them. In the facet of research, because I was mainly focused on experiment in Japan, the theory calculation in here is good for me to expand my view. Even I didn't got many results, but I believe the study of the basic quantum theory and modern simulation method on material will be useful for my future work.

Acknowledgement

I would like to appreciate Professor Jane P. Chang for giving me the opportunity to study in her group. Her guidance, valuable advices allowed me to progress in my understanding of this research. I also would like to deeply thank Calvin Pham for collaborating and giving valuable advices on this work. A big thanks to members of Prof. Chang's group, Dr. Taeseung Kim, Dr. Ya-Chuan (Sandy) Perng, Vladan Jankovic, Nathan Marchack, Jea (Jay) Cho, Diana Chien,

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