

Proposal for IGERT Capstone Course  
Spring 2008  
Alfred Lee – Physics (de Lozanne)  
Capstone advisor: Demkov

## 1 Objective

As my main research focus is centered around Scanned Probe Microscopy (SPM) techniques, it is easy for me to become engrossed in the technical matters surrounding the construction and operation of these instruments. To avoid losing sight of the physics behind my work and also in the spirit of the IGERT program, it is my intent to work with Professor Alex Demkov to model the behavior of one of the materials that I have been studying, namely the multiferroic  $\text{BiFeO}_3$  (BFO). A fair amount of work has been reported on which I hope to build. In working towards this goal, I will be forced to become more deeply familiar with solid state theory and current approaches to modeling complex metal oxides. This experience will undoubtedly improve the quality of my research in the future.

## 2 Background

One limiting factor to the density of magnetic memory storage is the long-range nature of the magnetic fields typically necessary for write operations. The ability to write bits using localized electric fields as opposed to extended magnetic fields would virtually eliminate this factor.  $\text{BiFeO}_3$  is a magnetoelectric multiferroic material exhibiting simultaneous and coupled ferroelectricity (FE) and antiferromagnetism (AFM) at room temperature and well above.[1] It is well known that the magnetization direction of a ferromagnetic (FM) material adjacent to an AFM material will be pinned by the ordering of the AFM domains. Furthermore, flipping the state of the antiferromagnet would cause the state of the ferromagnet to flip. Termed “exchange bias” this is indeed one of the enabling technologies of modern hard drives. A FM material adjacent to BFO would have its magnetization similarly pinned. The coupling between the FE and AFM orders in BFO would then allow the control of the FM magnetization through applied electric fields across the BFO layer.[2]

The coupling between FM and AFM phases has been demonstrated by Ramesh's group at Berkeley.[2] Our group is working with a patterned sample provided by this group to demonstrate active electrical switching of the magnetic domains. Our expertise in magnetic force microscopy (MFM) is invaluable here. We can observe the magnetic domain structure, apply a potential through the MFM tip, and observe any changes without causing any other changes to the sample in between. As we work towards this goal, I wish to engage in computational studies in order to better understand the behaviors of this material.

The local spin density approximation (LSDA) to density functional theory (DFT) was first used to model the electronic structure of multiferroic systems with limited success due to the localized electrons in these systems. Two computational methods have yielded more successful results: the LSDA plus Hubbard U (LSDA+U) method and the self-interaction corrected pseudo-potential method (pseudo-SIC). These were able to reconcile a disagreement on the magnitude of the spontaneous polarization of bulk vs. thin film BFO samples as well as explain the observed weak ferromagnetism in this primarily antiferromagnetic material.[1] Later work using the generalized gradient approximation (GGA) was able to produce several results that agree well with experiment, including structural parameters and polarization direction. Since the GGA tends to give better structural parameters, it may be more useful for considering FE properties[3]

### **3 Research Plan**

Some time must be spent familiarizing myself with the features and physical justifications of the various models in use. I must also learn to use software packages such as VASP or OpenMX as well as the TACC system. I have chosen to use OpenMX since it is an open-source package with broad functionality and is well documented. The course of my education will involve reproducing old results such as properties of silicon, iron, etc. in order to learn the software's interface as well as reading texts to learn the theory.

Once comfortable, I will attempt to reproduce the results of previous calculations of BFO. I plan to start with the simpler, though insufficient, LSDA, then the LSDA+U, then the GGA approximations. Eventually I would like to model the exchange interactions which lead to the pinning of an adjacent FM layer. Quantities of interest here are the amount of enhancement of the coercivity and the dependence of the effect on the thicknesses of the BFO and FM layers. Also, a measure of the length scales of the domains would be interesting to compare to experiment. Though an admittedly very ambitious plan, the prize is in the experience. To reach these latter goals as stated may take several semesters of more work which is not beyond me to attempt.

I expect to spend 8-10 hours distributed through the mornings of every week working on this project. What computational work can be done on a desktop will be performed using my personal computer at home. This can be done without interfering with my usual lab work. Any necessary supercomputer time at TACC will be discussed with Professors de Lozanne and Demkov. I will meet with Professor Demkov once a week to discuss my progress. I will also plan to attend Professor Demkov's group meetings to further my education.

### **4 Milestones and Questions to Answer**

Compute silicon structure, band structure, etc.

Compute cobalt or iron spin-dependent band structure and total magnetization.

Simulate bulk BFO.

-Find equilibrium structure given simple perovskite structure as a starting point.

-Try LSDA first, but move on to LSDA+U.

-Try expanding unit cell.

-Calculate spontaneous polarization.

-Calculate magnetization.

Simulate thin film BFO/ferromagnet interface.

### **5 Budget**

Costs for this project are expected to be minimal or absent, limited to the cost of TACC time.

### **6 Final Report**

We have agreed that I will demonstrate my results at the end of the term through a short project report and accompanying presentation.

## 7 References

1. C. Ederer, N. A. Spaldin, *Recent progress in first-principles studies of magnetoelectric multiferroics*, *Current Opinion in Solid State and Materials Science*, **9**, 128-139 (2005)
2. Y.H. Chu, R. Ramesh, et al., *Electric-field control of local ferromagnetism using a magnetoelectric multiferroic*, preprint
3. P. Ravindran, R. Vidya, A. Kjekshus, H. Fjellvåg, O. Eriksson, *Theoretical investigation of magnetoelectric behavior in BiFeO<sub>3</sub>*, *Physical Review B*, **74**, 224412-224429 (2006)