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The novel phenomenon of spin strain coupling in $BaTiO_3$

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1 Abstract

We have chosen $BaTiO_3$ for studying the relationship between the applied strains and the electron exchange by first principles computations done with Crystal09 [1]. We have found an evidence of the coupling between the applied lattice strains and the possible spin exchange in a cubic and tetragonal phase of $BaTiO_3$. The variation in the electron exchange energy depends upon the type of the strain, crystalline symmetry of the material and the atomic orbital overlap of the constituent atoms for the particular direction of the applied strain.

2 Introduction

For the cubic $BaTiO_3$, the application of the axial strains result in a linear increase in electron exchange energy if the strains are are applied in small steps within the limits of Hook's law. The strains are systematically applied in 7 steps of 0.005 value around the equilibrium lattice distance of 4.01 Angstrom. For the axial strains, the electron exchange energy has increased linearly with the expansion in the lattice strains. The increase in strain favors the indirect spin exchange interaction between the spins of the electrons in Ti and O atomic orbitals in a cubic $BaTiO_3$. The cubic BaTiO3 is a ferroic material as it may have changed to a ferromagnetic phase when it is strained.

The advent of the new materials and technologies is imminent as the device dimension of CMOS is approaching the size of an atom. The decrease in the transistor size and an increase in the device density on a chip has brought the Si based micro fabrication industry to an important juncture in the history of the semiconductor micro fabrication. The birth of the new

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materials [2, 6], fabrication technologies and device topologies [3, 4, 5] is the direct consequence of the advancements in the Si micro fabrication industry. This new era is full of the opportunities and challenges associated with the novel emerging technologies like spin based logics [9], bio inspired materials and molecular electronics. The important paradigm shift in the research methodology is emerging as the gap between the micro fabrication industry and the computational material physics [1] is narrowed down by the success of sub 100 nm Si CMOS as a switching device. The consequential increase in the computational speed of the processor, leading to the immense success in computational physics modeling, is attributed to the advancement in the Si micro fabrication techniques.

An other very important scientific and technological development has also taken place in the last few years that has also widely impacted the Si material physics research and the micro fabrication industry. It is the single most success of the magnetoresistance based spin logic. The important change has facilitated the coordination between Si semiconductor micro fabrication technology and the new spin logic devices [7] based on the composite thin film interfaces [2] of the metal. The spin of the electron in a transition metal is exchange-coupled [8], [10],[11], with the nearest neighbor atoms in the composite thin films. The charge transport in a direction lateral or transversal to these composite thin films, of the transition metal and thin metal or insulator layers, results in the giant magnetoresistance (GMR) and trans magnetoresistance (TMR). The advent of TMR and other spin based devices has brought the ultra thin film surface interfaces [2] at the fore front of the research on the new materials and technologies. The new material properties like GMR and TMR are based on the interactions arising purely due to the surface interactions [6] along the composite thin film structures. This is a big transition from the bulk materials after the first success of the surface interface of Si and its oxide for the realization of the CMOS transistor as a switch. The spin logic can perform at the room temperature in coordination with the Si based devices and systems.

The spintronics technology is not completely liberated from the electron charge transport as the separation requires a high band gap magnetic material having the spins spontaneously polarized at the room temperature. The search for this novel material with the spins spontaneously polarized and free of charge transport led us to the oxides of the transition metals. But only a few of the transition metals, their oxides [7] and crystalline geometries are favorable for the spontaneous polarization of spins without any charge trans-

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port. The transition metal oxides have the sufficient band gaps supported by the net spins localized due to d orbitals. The spin exchange coupling can help in the injection, transport and detection of the charge less logics. The transition metal and their oxides are fascinating and possess very complex material properties. They are challenging materials as the fabrication of these materials is challenging. Fortunately, the crystalline geometry of these ceramic materials, obtained with the thin film sputtering and deposition methods,is useful during the testing and characterization of these materials.

The oxides of transition metals may be understood better if they are analyzed by computational physics simulations done with the first principles techniques. The interactions across the thin film surface interfaces are mainly strain based and the understanding of the materials and property relationships is very vital. The computational results of the elastic constants, bulk moduli are done for the bulk and surfaces of the transition metal oxides.

3 The spin strain exchange coupled logic

The charge less spin exchange based logic is intimately coupled with mechanical properites. The change in the strains determine the change in the spin exchange energy. The computation of mechanical properties are completed for the cubic and tetragonal $BaTiO_3$. The next important phase is to investigate the details of the complex dependence of the electron exchnage on the elastic strains. There is a complex dependence of the electron exchange depending upon the nature of the applied strain and the crystalline symmetry of the material. For the cubic $BaTiO_3$, the electron exchange energy is increased linearly for the axial strain. The axial strains are applied in systematic and well-defined smaller steps. For the axial strains in a cubic $BaTiO_3$, It has been observed that there is an increase in the electron exchange energy [11] as the as the distance between the atoms is increased and the decrease in the exchange energy with the decrease in the distance between the atoms. Where as for the transversal strain the electron exchange energy increases for the expansions as well as the reduction of the unit cell volume. The complexity of the electron interaction is a direct consequence of the atomic overlap of the p and d atomic orbitals of Oxygen and Ti atoms. In case of the axial strains the overlap of the atomic orbital enforces the linear increase and decrease in the electron interaction depending upon the position of the deformed atomic orbital overlap. In case of the off-diagonal or transversal

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strains the p-d orbital overlap enforces the decrease in the electron exchange energy for expansion as well as the reduction in the unit cell volume of the cubic $BaTiO_3$. The spin exchange depends upon the energy of the exchange as well as the position of the atoms [11]. in both cases we see that the position of atoms is changed and the electron exchange energy is lowered [8]. The lowering of the electron energy may lead to the spins alignment.

4 Importance of ab-initio computations for materials, devices and systems

The success of the new materials, device topologies and the fabrication technologies supporting the Si based semiconductor micro fabrication industry is partially attributed to the computational physics techniques. The reduction in device sizes supported by the Si based semiconductor micro fabrication, the superb material properties, and its oxide has brought forward this new characteristic which was not as dominant until now. The computational physics has now become a new tool to compute the material properties like band gap and density of states brought forth by large growth in the computational power.

The new materials, device topologies and technologies are emerging because of the computational physics. The bulk and surface interfaces are one of the new frontiers of the material physics and the computational physics has succeeded in forecasting the material properties based on the crystalline geometry and the atomic orbitals for the unit cell of the periodic crystalline geometry. The extraction of the the novel physics of the materials at the surfaces, interfaces and phase boundaries is made possible by the success in the computation of the ground state energy. The experimental results have confirmed the essence of these computational techniques. With the success in the computational results we can move forward to fabricate the materials and test and characterize them to verify the resulting properties further. This comparison is being done for the polymers, organics, ceramics, transition metals, alkalines, lanthanides and their oxides.

5 Computational results

We are reporting the lattice strains and the electron exchange energies for the cubic BaTiO3. The lattice strains are applied in the systematic steps around

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the equilibrium lattice constant of 4.01 Angstrom. We have found a complex relationship between the variation in the electron exchange energy and the lattice strains. We are reporting the axial strains and the changes in energy for the cubic $BaTiO_3$. There is a linear increase in the electron exchange energy when the unit cell volume is expanded as reported in Table 1. In case of of the transversal strains we have seen the decrease in the electron exchange energy for the expansion as well as the reduction of the unit cell volume. The figure 1 reports the unit cell expansions and reductions in the systematic manner and the resulting changes in the total energy in Hartree units. The results of the electron exchange are shown in Figures 2 and 3. The E_{e-e} is the electron exchange energy and Et is the total energy in Hartree units. We performed the HF computations on cubic BaTiO3 to check the electron exchange and the total energy for the spins to be spontaneously polarized. We found the values of the total energy E_{total} and the electron exchange energy E_{e-e} of 352.9694787 and 50.531521 Hartree. The value of 1 Hartree equals 27.21 eV. The comparison of the values of total and electron exchange energy resulting from the strains with these values we have observed that the increase in the values of the total energy and the electron energy is sufficiently lower than the values of 352.9694787 and 50.531521 Hartree. However it suggests that we are approaching towards the possibility of the spin alignment as the unit cell volume is expanded.

6 Conclusions

The evidence of the coupling between the electron exchange and the lattice strain has been fund in cubic $BaTiO_3$. The electron exchange energy varies in a complex manner depending upon the strain applied in axial or transversal direction and the type of the crystalline geometry of the material. We have observed the linear increase in the electron exchange energy with the increase in the strain in the axial direction of the cubic $BaTiO_3$. However, there is a decrease in the electron interaction energy when the strains are applied in transversal directions. The comparison of the values of the total and the electron exchange energy with the spin polarized values of the total energy and the electron energy suggests that we are approaching closer to the values of energy required for the spin alignment. So the $BaTiO_3$ is a ferroic material which may change to ferromagnetic when it is strained.

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Tab. 1: The comparison between the strains, total energy, the coulomb energy and the exchange correlation energy during application of small strains

a	E_{total}	E_{e-e}
3.975	-307.533532	38.866100
3.980	-307.534548	38.952256
3.985	-307.535383	39.039733
3.990	-307.536081	39.128399
3.995	-307.536612	39.218338
4.000	-307.536996	39.309494
4.005	-307.537240	39.401846
4.010	-307.537352	39.495395
4.015	-307.537337	39.590058
4.020	-307.537202	39.685875
4.025	-307.536953	39.782814
4.030	-307.536595	39.880849
4.035	-307.536135	39.979960
4.040	-307.535577	40.080135
4.045	-307.534926	40.181357

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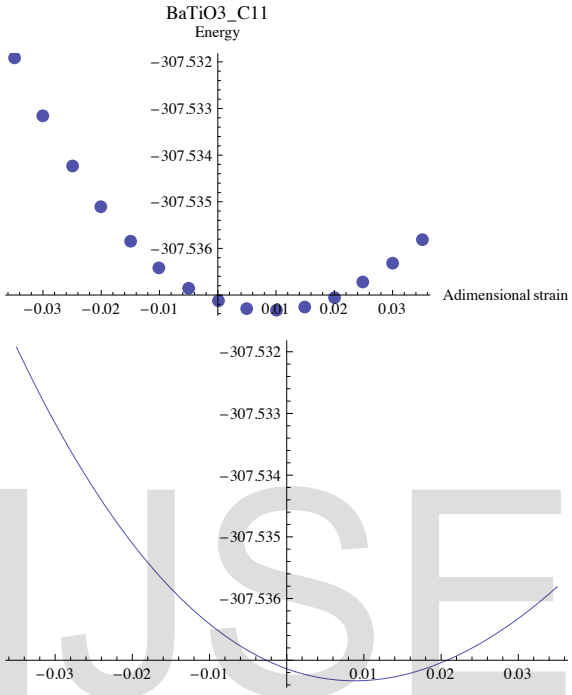

Fig. 1: The asymmetric strain-Energy (Hartree) computational results are obtained with ab-initio Hartree Fock computations done on cubic $BaTiO_3$. The filled circles show the computational results. The line graph shows the fitting results.

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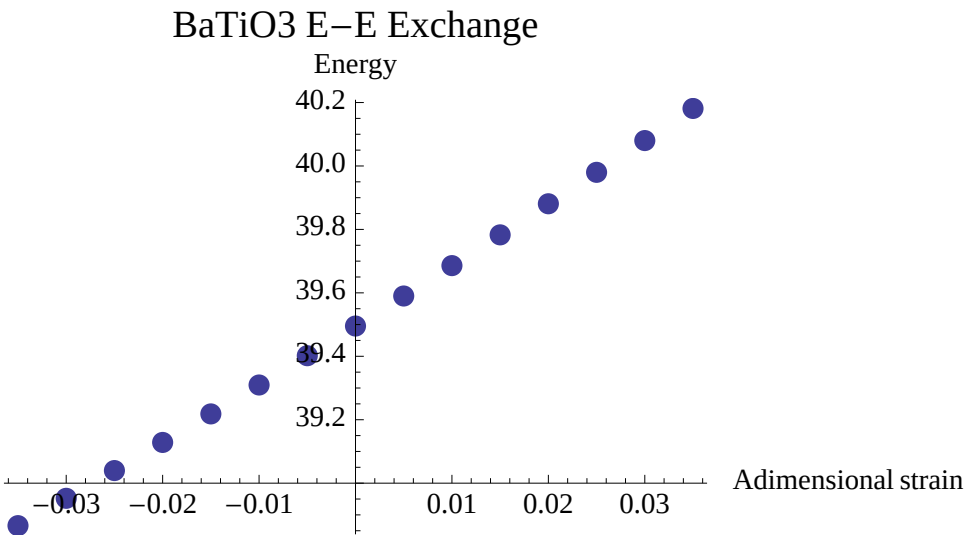

Fig. 2: The strain vs. Electron-Electron energy (Hartree) results are obtained with ab-initio Hartree Fock computations done on cubic $BaTiO_3$. The filled circle depict the data points.

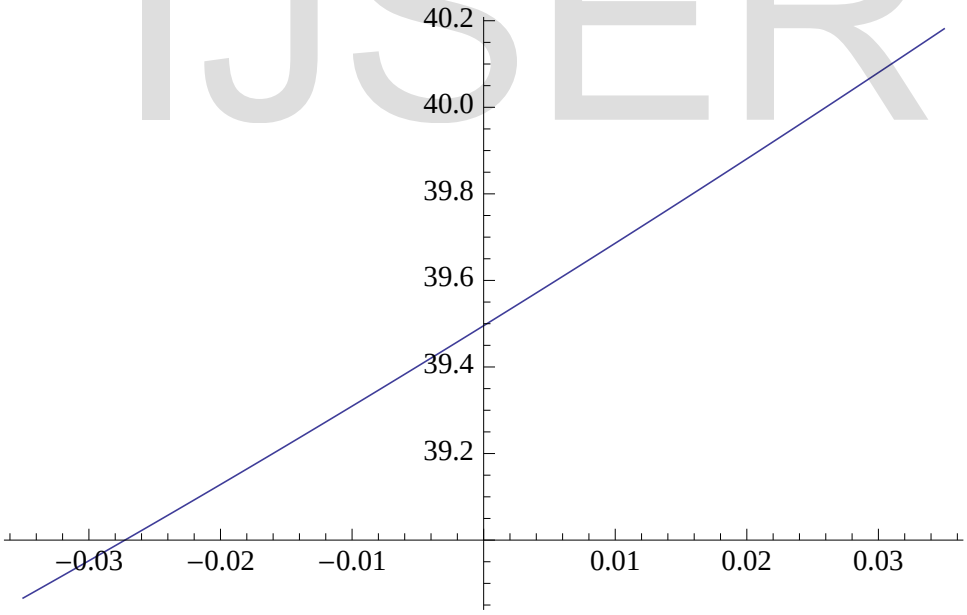

Fig. 3: The strain vs. Electron-Electron energy (Hartree) results are obtained with ab-initio Hartree Fock computations done on cubic $BaTiO_3$. The line graph shows the fitting results.

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