Manganites Superlattice

Xiaotian Zhang(xzhang25@utk.edu)

Instructor: Elbio Dagotto

Class: Solid State 2, 2010, Spring semester

Department of Physics and Astronomy

The University of Tennessee, Knoxville, TN 37996, USA

(Dated: Feb.16th.2010)

Abstract

A brief introduction on the Manganites family and recent work on superlattices will be produced. In this article, I will show some recent theoretical results and what will be the main point to do in the coming days about the superlattices.

I. THE MANGANITES

A. What is Manganites

Manganites means the oxides of Mn, typically have the form of $AMnO_3$ with the perovskite structure. In this picture, the red spheres are the A atoms, which usually belong to

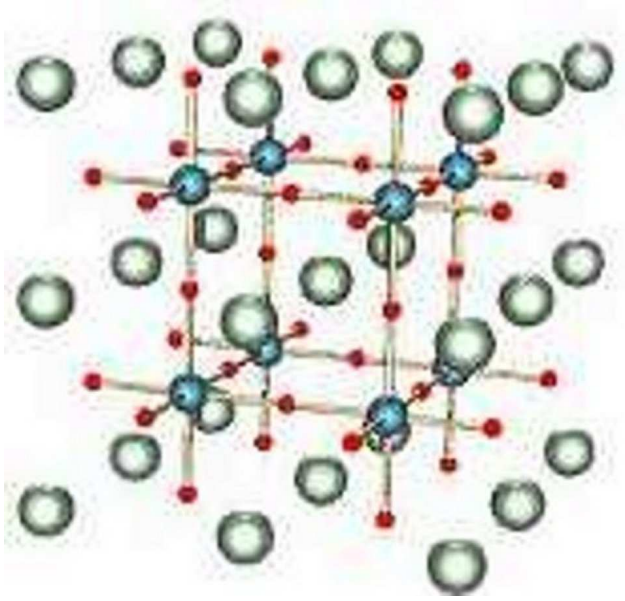

FIG. 1: Peroxskite structure

the rear-earth elements or the Lanthanide series. The blue balls are Mn atoms while the green ones correspond to the oxygens.

B. Why Manganites

As an important branch of the strongly correlated electronic systems, manganites has been studied both theoretically and experimentally for more than half a century, and is still a hot topic today. Some of the reasons can be explained as the following[14578]: 1. The unexpected large magnetoresistance: Colossal MagnetoResistance (CMR)[6], which has up to more than 100000% MR. As we all know, another type of MR, the giant magnetoresistance (GMR), already has great industrial applications and led to a Nobel Prize. Naturally, there are many people think that the manganites with the CMR effect will be as good as, even better than, the GMR materials, although they still need to enhance the Curie temperature

beyond room temperature, and lower the needed magnetic field to some practical value.

2. The rich phase diagrams and phase separation: People have found varieties of phases

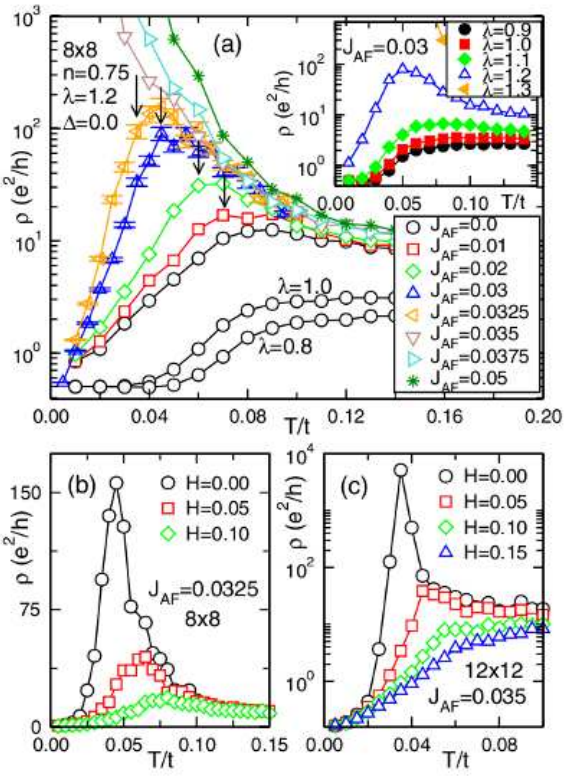

FIG. 2: Numerical results of CMR.(Sen et al)

in the manganites family, showing interesting properties in spin, charge, and orbital order. What's more, different phases can co-exist and compete with each other in the same bulk. This competition will lead to properties different from those in the single phase materials. For example, the competition of the charge ordering (CO) phase and the ferromagnetic (FM) phase is widely believed to be the origin of the CMR effect.

C. Goes to the superlattice from the past

After detailed studies for more than half a century, the properties of the bulk manganites are well concluded and most of them are already understood. On the other hand, in the bulks, the CMR effect is of great interest but still far away from applications due to the required temperature and magnetic field. So, the manganite superlattices came into the

sight of people for both physical and practical reasons.

D. Microscopic Double-Exchange Model

The theoretical model is the double exchange model, which I already explained in the first oral presentation, but here we need a small correction. Due to a superlattice is not translational invariant, the electric potential energy of an electron is dependent on the position of the electron:

$$\begin{aligned} H = & \sum_{i,j,\alpha,\beta,\sigma} t_{i,j,\alpha,\beta}\Omega_{i,j}c^{\dagger}_{i,\alpha,\sigma}c_{j,\beta,\sigma} + \sum_{i,j} J_{AF}\vec{S_i}\cdot\vec{S_j} \\ & + \sum_{i}[\lambda(-Q_{1,i}I_{2\times 2} + Q_{2,i}\tau^x_i + Q_{3,i}\tau^z_i) + \frac{1}{2}(\gamma Q^2_{1,i} + Q^2_{2,i} + Q^2_{3,i})] \\ & + \sum_{i,j}\vec{D_{ij}}\cdot\vec{S_i}\times\vec{S_j} + \sum_i e\phi_i n_i \end{aligned} \tag{1}$$

in principle, the staticelectric potential ϕ_i can be expressed by the Maxwell equation

$$-\nabla^2\phi_i = 4\pi n_i \tag{2}$$

and we need to iterate the above equation and the Hamiltonian in order to obtain the correct result. However, most of the calculation time is spent on the diagonalization of the matrices, so that if we need to do 100 times iteration for each configuration of the lattice, the time needed for a superlattice will be about 100 times longer than that for a bulk with the same lattice size, which is not affordable.

In practice, we only consider the potential produced by the nearest A ions. For example, if there are 2 kinds of A ions a and b, then a site between a and a ions will be set to have a potential equals to 0, while a site between b and b ions has a potential V. Naturally, a site between a and b ions should be considered with potential V/2. This kind of trick, which indeed will lower the accuracy of the calculation a little bit, significantly reduces the time people spend on the work.

II. SOME EXPERIMENTS DONE FOR THE SUPERLATTICE

A. LMO:SMO=1:2

In such systems, it is shown clearly that there is a significant transition at $m = 3^9$.

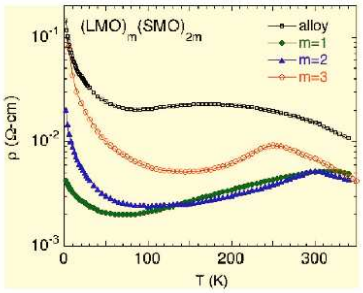

FIG. 3: Resistivity

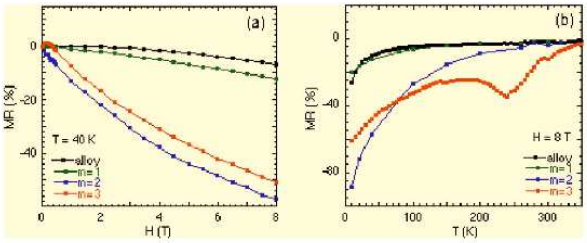

FIG. 4: Magnetoresistance

B. LMO:SMO=2:1

For 2 : 1 systems, only a tiny abnormal MR is found with the increase of m.[10]

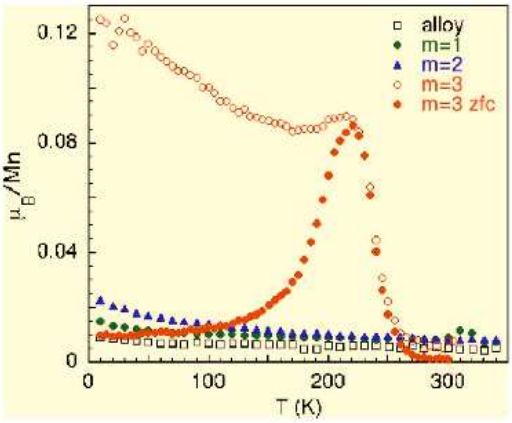

FIG. 5: Magnetization

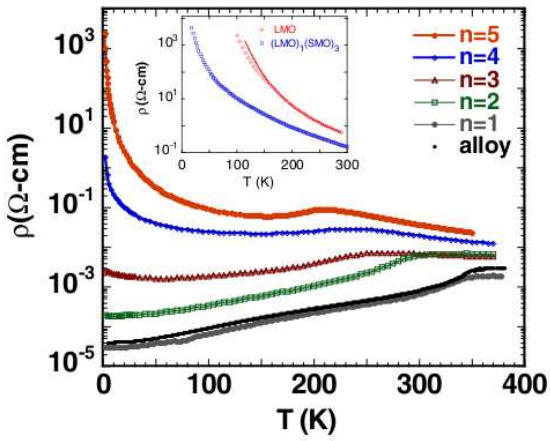

FIG. 6: Resistivity

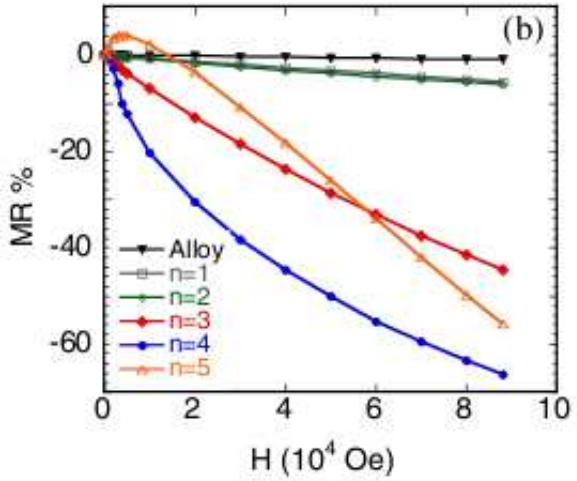

FIG. 7: Magnetoresistivity

III. THEORETICAL WORK FOR THE SUPERLATTICE

A. LMO:SMO=2:1

Shuai Dong has already done some work for the system with LMO:SMO=2:1 and obtained many results of the spin order, orbital order, charge order and conductivity. They are shown by the following pictures.[2]

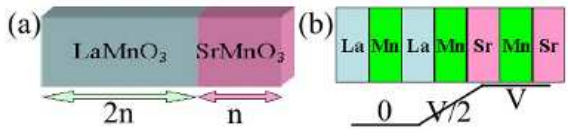

FIG. 8: LMO/SMO

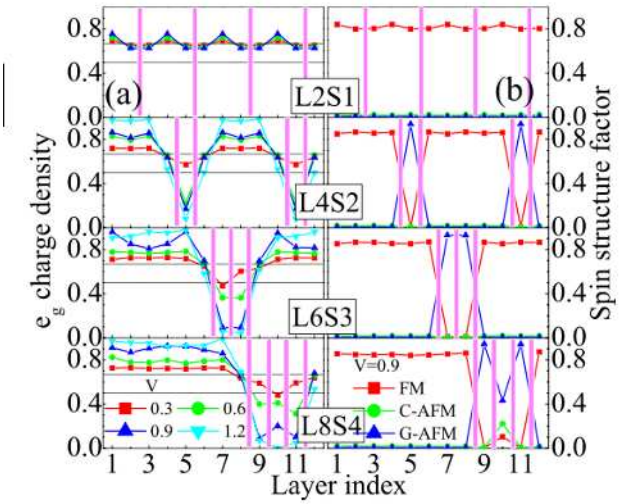

FIG. 9: Charge and Spin Order

B. The Future

In the future theoretical study, we are going to explore more beyond the 2:1 superlattice, for what some experiments are already done.[3] In theory, the main difficulty is the effect of tension. It is evident that at the interface of layers with different A ions, the tension will

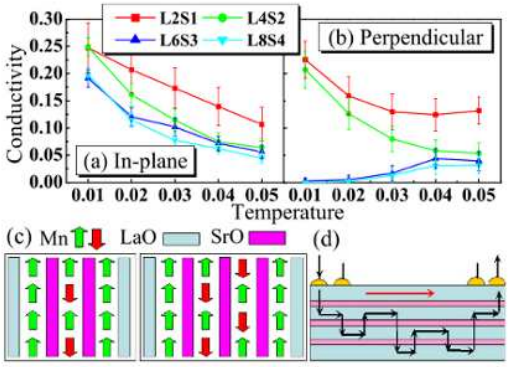

FIG. 10: Conductivity and In-Plane Spin

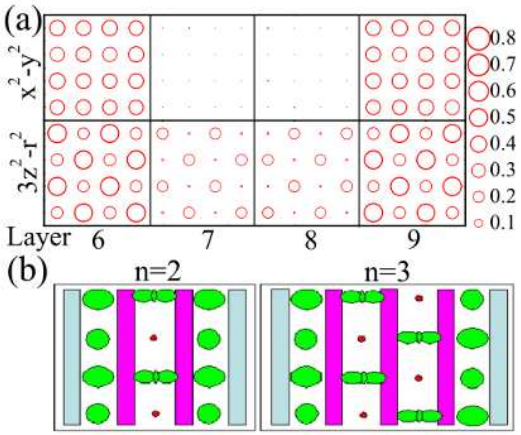

FIG. 11: Orbital Order

distort the superlattice from the perfect cubic structure so that we need to consider the displacement of the Mn atoms.

These displacements will, on one hand, affect the hopping and super exchange amplitudes, which will be anisotropic and site dependent now. This will of course introduce a huge number of parameters to judge in a numerical work.

On the other hand, the displacement of the Mn atoms will lead to site dependent intrinsic distortion of the Oxygens. This can be done manually by initializing the configuration with

the distortion observed by experiment.

What's more, the Jahn-Teller modes in the above double exchange model are only the 3 linear modes ($Q_1 - - - Q_3$). There are other 3 rotation modes ($Q_4 - - - Q_6$) which can also be important in the present of tension. If this is the case, both analytical and numerical work for these 3 modes are required.

Another point is, in the numerical calculation, the size of the superlattice must not be smaller than one period of the real superlattice under the periodic boundary condition. This can easily give a very large lattice size, which costs people a lot of time in front of a computer.

IV. SUMMARY

As a raising field, the manganite superlattice is of great interest both in physics and industrial applications. Experiments are keep running to explore the properties of such structures, while theorists are also making efforts to understand the same thing. And the main theoretical challenge today is how to describe this complicated system with the double exchange model as simple, compared with the ability of the computers , as possible.

---

[1] E. Dagotto, et al Nanoscale Phase Separation and Colossal Magnetoresistance ISBN 3-540-43245-0 (2002).

[2] Shuai Dong, et al PRB, **78** 201102 (2008).

[3] T. S. Santos, et al Not published.

[4] E. Dagotto Sience **309**, 257 (2005).

[5] E. Dagotto New Journal of Physics **7**, 67 (2005).

[6] C. Sen, et al PRL **98**, 127202 (2007).

[7] E. Dagotto Sience **318**, 1076 (2007).

[8] E. Dagotto and Y. Tokura. MRS BULLETIN **33**, 1037 (2008).

[9] A. Bhattacharya, et al Appl Phys. Lett **90**, 222503 (2007).

[10] A. Bhattacharya, et al PRL **100**, 257203 (2008).