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Strong correlation between lattice strains and Curie temperature in $La_{1-x}(Ca/Sr)_xMnO_3$

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Abstract

Atomistic simulations have been performed on $La_{1-x}(Ca/Sr)_xMnO_3$ to investigate the lattice strains effect on Curie temperature T_C upon doping or under pressure. It is found that there is a strong correlation between T_C and the lattice strains introduced by doping or pressure. This founding agrees with the results given by Millis et al. [A.J. Millis, T. Darling, A. Migliori, J. Appl. Phys. 83 (1998) 1588] and Tsui et al. [F. Tsui, M.C. Smoak, T.K. Nath, C.B. Eom, Appl. Phys. Lett. 76 (2000) 2421], there was a strong correlation between T_C and the lattice strains introduced by substrate mismatch. It is also found that there is a correlation between Curie temperature and local lattice structures (Jahn–Teller distortions). We propose that these two types of correlations we used may have some intrinsic relations.

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Keywords: Colossal magnetoresistance; Manganites; Lattice strains; Curie temperature

1. Introduction

The doped manganites have been a hot topic in condensed matter physics from 1990s for at least two reasons. Firstly, these compounds manifest colossal magnetoresistance (CMR) around Curie temperature T_C with a potential application in magnetic memory industry [1–3]. Secondly, some interesting phenomena are found: charge ordering, Jahn–Teller effect [4], phase separation [5,6], etc.

After the founding of CMR, the correlation among composition, lattice structure, and properties of doped manganites were investigated. It is found that the radius of doping ion has important effect on Curie temperature as illustrated by the so-called double exchange mechanism [1,2]. Some theoretical [7] and experimental [8] results indicated that T_C exhibits strong correlations with substrate-induced strains in manganite films, which contain bulk and Jahn–Teller components. This method has been used to discuss the electromagnetic properties of doped manganites on different substrates [9,10]. Zhao et al. [11] proposed a formula $T_C \propto W_{eff} \propto W \exp(-\gamma E_{JT}/h\omega)$ to qualitatively explain the Jahn–Teller energy E_{JT} dependence of T_C. Radaelli et al. [12] believed that E_{JT} influence on T_C in $A_{1-x}A'_xMnO_3$ cannot be ruled out, and 20% change in E_{JT} will result in a comparable T_C variation.

Although above work had given important clues to understand the lattice structure dependence of magnetic properties, especially of T_C, there are still some uncertainties to be considered. Firstly, to our knowledge, not only the substrate mismatch but also doping and pressure can introduce lattice strains in manganites, maybe these strains have the same effect on T_C. Secondly, doping or pressure can introduce both inner structural transitions by Jahn–Teller distortion and outer structural transitions (the changes in lattice parameters). It is necessary to compare these two types of lattice transitions and their effects on T_C. In order to discuss above two questions, we perform systematic atomistic simulation on $La_{1-x}(Ca/Sr)_xMnO_3$ and investigate the correlations between lattice strains and T_C.

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2. Atomistic simulation method

Our atomistic simulation, based on the widely used successful Born core-shell model [13], can predict the crystal structure of a compound at a given temperature and pressure by minimizing its free energy. It has been used for investigate the structural transition and atomic distribution [4,14,15] in Ca/Sr- and Co/Ni-doped manganites. A brief illustration of this technique is available in [14].

As atomistic simulation is strongly depending on the validity of the potential model used, we have checked the reliability of the potential used in this work. The potential parameters of $LaMnO_3$ and $CaMnO_3$ can reproduce the experimental crystal structure of $LaMnO_3$ or $CaMnO_3$ with the differences in lattice parameters between the calculated and experimental data less than 1.0% [14]. We have calculated pressure effect on $LaMnO_3$ up to 3.4 GPa for further testing these potential parameters. When pressure is less than 3.5 GPa, the calculated compressibility of V, a, b, and c are $10.0\times10^{-3}\,\mathrm{GPa}^{-1}$, $9.0\times10^{-3}\,\mathrm{GPa}^{-1}$, $-0.12\times10^{-3}\,\mathrm{GPa}^{-1}$, and $1.1\times10^{-3}\,\mathrm{GPa}^{-1}$, respectively. The corresponding experimental values are $8.1\times10^{-3}\,\mathrm{GPa}^{-1}$, $6.1\times10^{-3}\,\mathrm{GPa}^{-1}$, $0.96\times10^{-3}\,\mathrm{GPa}^{-1}$, and $1.3\times10^{-3}\,\mathrm{GPa}^{-1}$, respectively [14]. The calculated results of the compressibility are in agreement with the experimental results except for the compressibility of the lattice parameter b, indicating that the potentials we used can represent the crystal structure of $LaMnO_3$. We have also investigated the temperature effect on $La_{1-x}(Ca/Sr)_xMnO_3$ and found that the potentials are stable and suitable at low temperature (<100 K). Above lattice, pressure, and temperature effect checks indicate that our potentials can represent the interaction between ions in Ca/Sr-doped $LaMnO_3$.

3. Results and discussion

3.1. Lattice distortion

For $La_{1-x}(Ca/Sr)_xMnO_3$, about 16–200 doping configurations have been simulated at every doping density. It is noticed that the converged configurations of $La_{1-x}(Ca/Sr)_xMnO_3$ always have the character of clustering or charge ordering ($x=0.25$ or 0.33), i.e., Ca^{2+}/Sr^{2+} or Mn^{3+}/Mn^{4+} ions form clustering local structure or charge ordering stripes [1,14–16]. We calculated the variations in the lattice parameters of $La_{1-x}Ca_xMnO_3$ ($0\leqslant x\leqslant 0.33$) [17] that agree with the experimental data [18,19]. If we use the differences between the three lattice parameters $(a, b/\sqrt{2}, c)$ to present the magnitude the lattice distortion, one can find that the lattice distortion of $La_{1-x}Ca_xMnO_3$ ($0\leqslant x\leqslant 0.33$) decreases as doping density increases. For Sr-doping, our calculated lattice parameters [17] also approximately agree with the experimental data [19–21]. At Sr doping density $x=0.25$, the lattice distortion almost disappears.

We studied pressure (≤4.5 GPa) effect by using one converged configuration of $La_{0.75}Ca_{0.25}MnO_3$ and $La_{0.89}Sr_{0.11}MnO_3$. The simulated results are shown in Fig. 1. For $La_{0.75}Ca_{0.25}MnO_3$, as pressure increases from 0 to 4.5 GPa, lattice parameters a and c decrease significantly, but b decreases a little (Fig. 1a). For $La_{0.89}Sr_{0.11}MnO_3$, as the pressure increases from 0 to 4.5 GPa, lattice parameters a and c decrease significantly, and b increases a little (Fig. 1b). As pressure increases, the lattice distortions of $La_{0.75}Ca_{0.25}MnO_3$ and $La_{0.89}Sr_{0.11}MnO_3$ also decrease just as that in $LaMnO_3$ upon Ca/Sr doping [17]. The structural transitions of CMR manganites upon doping and under pressure must affect their electromagnetic properties.

3.2. Lattice strains and T_C

Curie temperature T_C is an important property parameter for doped manganites, as their CMR effect always takes place near T_C. To our knowledge, there have been at least two influential methods for discussing the dependence of T_C on lattice transition in the CMR materials.

One method took into account the substrate-induced strains effect on T_C in manganite films. Millis et al. [7] deduced the dependence of T_C on strains by mean field theory and Tsui et al. [8] rewrote it as:

$$T_C(e_b, e_{JT}) = T_C(0,0)(1-\alpha e_b-\beta e_{JT}^2). \quad (1)$$

In this expansion the respective coefficients for the strains are $\alpha=\frac{1}{T_C(0,0)}\frac{dT_C}{de_b}$ and $\beta=\frac{1}{2T_C(0,0)}\frac{dT_C}{de_{JT}}$. In the films, since the substrate induces an even-parity strain symmetry in the growth plane [8,9], the observed three dimensions strain states by symmetry can be decomposed into a bulk strain:

$$e_b = 2e_{100}+e_{001}, \quad (2)$$

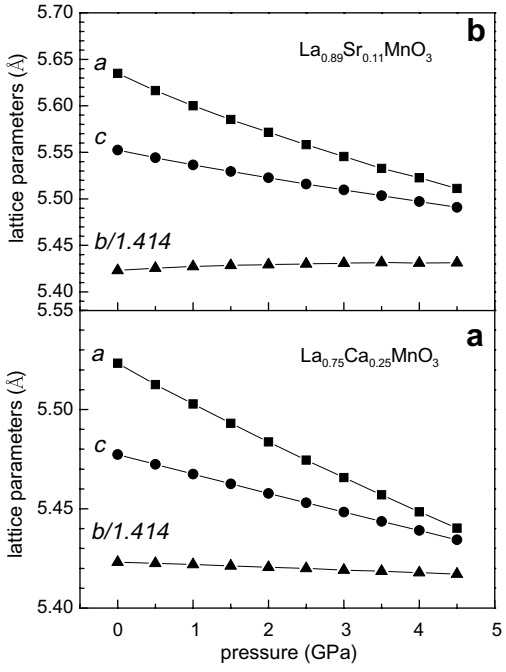

Fig. 1. Lattice parameters of $La_{0.75}Ca_{0.25}MnO_3$ (a) and $La_{0.89}Sr_{0.11}MnO_3$ (b) as a function of pressure (≤4.5 GPa).