Basic Mechanism and Potential Application of Ferroelectric Quantum Phase Transition: The Representative Case of $SrTiO_3$

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1. Introduction

The future trends of electronic devices are faster, lighter, and smaller. Ferroelectric with nanoscale domains is promising for data memory devices with ultrahigh density. Reduced operating temperatures can lead to lower leakage currents and to increased breakdown fields, both crucial for keeping competitive with faster access and high-density needs.

In this research, we study the low-temperature ferroelectric quantum phase transition of $SrTiO_3$. $SrTiO_3$ is perfectly centrosymmetric in macroscopic scale in the whole temperature range. The local structure within the scale of several unit cells is unclear. At low temperature, $SrTiO_3$ possesses quantum paraelectricity with multitudinous physical properties, which attracts a lot of attention[1]. We use extended X-ray absorption fine structure (EXAFS) to study the local structure of $SrTiO_3$ and its doped variants ($SrTi^{18}O_3$ and $Sr_{1-x}Ca_xTiO_3$). The results show $SrTiO_3$ has a non-centrosymmetric local structure and the ferroelectric quantum phase transition of $SrTi^{18}O_3$ and $Sr_{1-x}Ca_xTiO_3$ was confirmed by investigating the relative vibration of the atoms. The small non-centrosymmetric local structure of $SrTiO_3$ and low-temperature phase transition can be used to manufacture electronic devices with special functions, such as radiation-hardness of ferroelectric memories, and array radar devices[2].

2. Experimental Methods

Temperature-dependent Ti *K*-edge EXAFS of $SrTiO_3$ (STO16) and $SrTi^{18}O_3$ (STO18) was conducted by transmission mode at beamline BM23 of ESRF. The same experiment of $Sr_{1-x}Ca_xTiO_3$ sample was conducted at beamline 9C of Photon Factory. temperature to room temperature. With the advantage of element-selecting EXAFS can directly measure the geometric information around the Ti ion. The temperature is controlled by using cryostat chamber with liquid helium supply. Three structural models of the local structure of the $SrTiO_3$ were created and compared. The rhombohedral model is the best model for its low-fitting r-factor.

3. Results

Fig.1 a shows the Ti off-center value along the [111] direction in rhombohedral model of $SrTiO_3$ and $SrTi^{18}O_3$. It is clear that the local structure of $SrTiO_3$ is not centrosymmetric comparing to the macroscopic structure. The Ti off-center value in both $SrTiO_3$ and $SrTi^{18}O_3$ are almost the same and around 0.1 Å. It should be noted that the off-center value is not dramatic change with temperature, which means order-disorder type phase transition may exist in $SrTiO_3$ and $SrTi^{18}O_3$.

The ferroelectric quantum phase transition of $SrTi^{18}O_3$ was indicted in Fig.1 b. The mean square relative displacement of $SrTi^{18}O_3$ was increased in the low-temperature phase transition region. The mechanism of this phenomenon is complex. We use the pseudo-Jahn-Teller effect to interpret the Ti off-center, which illustrates the Ti ion is in a double-well potential. The quantum paraelectric phase of $SrTiO_3$ is due to the quantum tunneling of Ti ion between the two bottoms of the double-well. In $SrTi^{18}O_3$, because the increased mass of oxygen, the tunneling effect is suppressed, which results in the Ti ion is settled at one side of the double. The ferroelectric phase occurs when the domains are produced along with the correlation of Ti ions.

Reference

[1] Rowley, S. E., et al. *Nat. Phys.*, **10** 367(2014).
[2] Chandra, P., et al. *Rep. Prog. Phys.*, **80** 112502(2017).

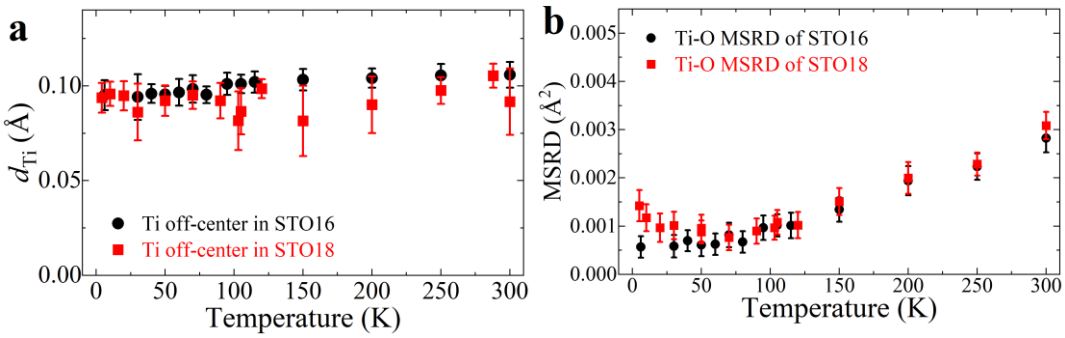

Fig.1 **(a),** Temperature-dependent Ti off-center value along the [111] direction in rhombohedral model of STO16 and STO18. **(b),** Temperature-dependent Ti-O MSRD of STO16 and STO18.