Investigation of electrical conductivity and dielectric properties of Sr$_2$FeTiO$_6$.

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Abstract. In this study, we use impedance spectroscopy in the frequency range of 5 kHz to 1 MHz and in the temperature range of 300–550 K in order to study the electrical conductivity and dielectric properties of Sr$_2$FeTiO$_6$. The dielectric constants show the classical type of the paraelectric state, with no pseudo relaxation peak. DC conductivity increases with increasing temperature according to the Arrhenius law, indicating a thermally activated process. The activation energy is evaluated based on the DC conductivity and using the Arrhenius equation. The relaxation mechanism is the same at various temperatures, as confirmed by the scaling of the imaginary part of the electric modulus.

Keywords: Sr$_2$FeTiO$_6$, conductivity, dielectric, impedance spectroscopy

1. Introduction
Double perovskite A$_2$B’B''O$_6$ offers a variety of properties depending on the combination of B’ and B”. It has numerous applications, such as solid oxide fuel cells (SOFCs), capacitors, sensors, and spintronic devices [1]. It also has promising high-temperature ferroelectric properties [2]. Double perovskite Sr$_2$FeTiO$_6$, which is a promising material for sensors and SOFCs, is composed of SrTiO$_3$ and SrFeO$_3$ [3].

Single perovskite SrTiO$_3$ is known for its quantum paraelectric properties, which are temperature-independent at very low temperatures (T ~ 3 K) [4]. SrTiO$_3$ is typically used as a resistance-based gas sensor. Many combinations of B’ and B” in perovskite SrTiO$_3$ have been studied in the search for enhanced properties of this n-type ferroelectric material. Doping SrTiO$_3$ with Fe decreases the band gap and increases the electron, hole, and oxygen-vacancy densities, leading to mixed ionic-electronic behavior [3], which makes this material suitable as an ideal gas sensor.

Based on previous research, the paraelectric state of Sr$_2$FeTiO$_6$ occurs at T >16 K. Lekshmi et al. [5] reported the dielectric properties and electrical conductivity of Sr$_2$FeTiO$_6$, for the temperature range of 200–300 K. In order to study the high-temperature properties of this material, we investigate its dielectric properties and electrical conductivity over the temperature range of 303–398 K.

2. Experimental
The Sr$_2$FeTiO$_6$ sample was prepared using the sol gel method. The experimental details are available in [6]. For IS characterization, the sample was pelletized and coated by carbon on both surfaces. The impedance was measured using an RLC meter over a temperature range of 303–523 K and a frequency range from 5 kHz to 1 MHz. Next, the sample was connected to a conducting probe and modeled as a parallel-plate capacitor. The RLC meter with a frequency range from 1 kHz to 1 MHz was used to measure the phase angle and the impedance of the samples as a function of temperature (293–523 K).
The real and imaginary parts of the permittivity, AC conductivity, and electric modulus are determined as follows [7]. The real part of the permittivity is

$$\varepsilon' = \frac{1}{\omega C_0} \left( \frac{Z'}{Z' + Z''} \right),$$

The imaginary part of the permittivity is

$$\varepsilon'' = \frac{1}{\omega C_0} \left( \frac{Z''}{Z' + Z''} \right),$$

with $Z'$ is the real parts of the sample impedance, and $Z''$ is the imaginary part of it, $\omega = 2\pi f$ and $C_0 = \frac{A\varepsilon_0}{\ell}$ is the vacuum capacitance.

The complex dielectric constant is

$$\varepsilon = \varepsilon' + \varepsilon''.$$  

(3)

The AC conductivity is

$$\sigma_{AC} = \varepsilon_0 \varepsilon'' \omega,$$

(4)

where $\varepsilon_0 = 8.854 \times 10^{-12}$ F/m is the permittivity in vacuum and $\varepsilon''$ is the imaginary part of the permittivity. The data are fit using the Jonscher power law (JPL):

$$\sigma_{AC} = \sigma_{DC} + A\omega^n,$$

(5)

where $\sigma_{DC}$ is the DC conductivity, $A$ is the temperature and material preexponential factor, the hopping frequency is $\omega = 2\pi f$, the frequency exponent is $n$ and $\sigma_{ac}$ is the AC conductivity. The value of $n$ ($0 < n \leq 1$) gives the degrees of freedom of the lattice and ions. The modulus is evaluated using

$$M' = j\omega C_0 Z',$$

(6)

$$M'' = j\omega C_0 Z''.$$  

(7)

3. Results and discussion

3.1. Dielectric properties

Figure 1a shows the dielectric constant of Sr$_2$FeTiO$_6$ as a function of temperature, which behaves as a classical dielectric in the range of 303–523 K. The paraelectric state, which is manifested by a linear
Figure 2. (a) Dielectric constant of Sr$_2$FeTiO$_6$ as a function of frequency. (b) Loss tangent of Sr$_2$FeTiO$_6$ as a function of frequency.

Figure 3. (a) AC conductivity as a function of frequency for various temperature, (b) DC conductivity as a function of inverse temperature at 303–398 K, (c) DC conductivity variation as a function of inverse temperature from 398 to 523 K.

increase in the dielectric constant with temperature, shows no relaxation peak. The dielectric type is confirmed by the shape of the inverse dielectric constant in each temperature (see the inset in figure 1a) and loss tangent as a function of temperature (figure 1b).

Figure 2a shows the dielectric constant of Sr$_2$FeTiO$_6$ as a function of frequency. The dielectric constant is large at low frequencies and becomes small and temperature-independent at high frequencies. A similar result was reported by Hzez [8], Pradhan [9], and Phoka [10]. This phenomenon is attributed to space-charge polarization.
The profile of frequency modulus (tendency the electric related to temperature) according to the Maxwell constant and so is actually a relaxation process in the electrode space charge polarization in the bulk and to the polarization process at the interfaces (electrode space charge) [13]. In the high-frequency region, the conductivity increases according to the power law $A\omega^n$, which puts it in the category of AC conductivity.

Figure 2b shows the loss tangent as a function of frequency. The dielectric loss ($\tan\delta$) exhibits a relaxation peak between 10 and 10 Hz at high temperatures (423–523 K). These peaks are attributed to the grain-boundary effect, which is a manifestation of the electrode-polarization effect [11,12]. The relaxation phenomenon only occurs at high temperatures because the grain-boundary effect is thermally activated.

### 3.2. AC conductivity

Figure 3a presents the logarithm of the AC conductivity in each frequency as determined by the Jonscher Power Law (JPL) in equation (5). At lower frequencies, the AC conductivity is relatively constant and so is actually a DC conductivity (see table 1). This phenomenon is attributed to Maxwell–Wagner space-charge polarization in the bulk and to the polarization process at the interfaces (electrode space charge) [13]. In the high-frequency region, the conductivity increases according to the power law $A\omega^n$, which puts it in the category of AC conductivity.

Given the temperature dependence of the electric parameters, the JPL gives $n$. At lower temperatures (303–398 K), the JPL is fully satisfied ($0 < n \leq 1$), which indicates a translational motion by hopping [14]. However, above 398 K, $n > 1$, which denotes localized hopping [14].

Figures 3b and figure 3c show the DC conductivity as a function of temperature. The DC conductivity was determined using the JPL. The activation energies determined by fitting to the JPL are 0.062 and 0.146 eV for translational hopping (figure 3b) and localized hopping (figure 3c), respectively.

### 3.3. Electric modulus

Figure 4a shows the real part $M'$ of the modulus as a function of frequency. The electric modulus is related to electric-field relaxation in materials when the displacement field is constant. Specifically, the electric modulus explains the relaxation process in the real part of the permittivity. $M'$ shows a tendency to increase with increasing frequency, the the value of M towards a constant value ($M \sim \infty$) at high frequency.

Figure 4b shows the imaginary part $M''$ of the modulus as a function of frequency. $M''$ exhibits a broad peak that shifts to a higher frequency as the temperature increases, which indicates that the relaxation rate increases with temperature. The region before the maximum imaginary part of the modulus ($M''_{\text{max}}$) reflects the long path of the charge carrier, and the region after the maximum frequency reflects the short path of the mobile charge carrier. The inset in figure 4b shows the scaling profile of $M''$. The fact that the curves overlap means that the relaxation at each temperature is based on the same mechanism.

### Table 1. DC conductivity and JPL exponent $n$ for various temperatures.

| Temperature (K) | DC conductivity (S/m) | $n$ |
|-----------------|-----------------------|-----|
| 303             | $9.22 \times 10^{-1}$ | 0.50|
| 323             | $1.65 \times 10^{-1}$ | 0.45|
| 348             | $2.79 \times 10^{-1}$ | 0.29|
| 373             | $5.74 \times 10^{-1}$ | 0.30|
| 398             | $1.17 \times 10^{-1}$ | 0.34|
| 423             | $2.38 \times 10^{-1}$ | 1.48|
| 448             | $4.08 \times 10^{-1}$ | 1.75|
| 473             | $6.83 \times 10^{-1}$ | 2.46|
| 498             | $9.56 \times 10^{-1}$ | 1.83|
| 523             | $1.41 \times 10^{-1}$ | 1.42|
Figure 4. (a) Real part $M'$ of the modulus as a function of frequency. (b) Imaginary part $M''$ of the modulus as a function of frequency. The inset shows the scaling profile of $M''$

4. Conclusions

Sr$_2$FeTiO$_6$ was prepared using the sol gel method. The dielectric constant of this material as a function of temperature follows the classical dielectric behavior in the paraelectric state. The AC conductivity fully satisfies the JPL in the temperature range of $303$–$398$ K. The thermal-energy-activated mechanism is confirmed by the increase in DC conductivity as the temperature increases and by the fit to the Arrhenius law.

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