Simultaneously improved dielectric, optical and conductivity properties of SrLa$_{1-x}$Nd$_x$LiTeO$_6$ double perovskites

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Abstract

In this study, SrLa$_{1-x}$Nd$_x$LiTeO$_6$ ($x = 0.00, 0.25, 0.50, 0.75, 1.00$) compounds were prepared using the solid-state method, and their structural, optical, dielectric and conductivity properties were investigated. The Rietveld refinement of x-ray diffraction (XRD) data shows that the compound crystallizes in monoclinic symmetry (i.e. $P2_1/n$ space group). The morphological scanning electron microscopy study reports a larger grain size when the dopant is added. The optical ultraviolet-visible light spectroscopy (UV-Vis) study reveals that the energy band gap decreases as the doping increases from $x = 0.00$ to 0.50. Dielectric studies using electrochemical impedance spectroscopy (EIS) characterization reveal the non-Debye trend of dielectric real permittivity ($\varepsilon'$) with the enhancement of $\varepsilon'$ at 1 MHz from $x = 0.00$ to 0.50. $\varepsilon'$ and the dielectric tangent losses (Tan $\delta$) show increment and decrement patterns, respectively, when the temperature is increased. The frequency-dependent conductivity ($\sigma_{AC}$) plot follows the universal power law at all temperatures, and the $\sigma_{AC}$ behavior in SrLa$_{1-x}$Nd$_x$LiTeO$_6$ is due to the tunneling of polarons.

1. Introduction

Perovskites with the ABO$_3$ configuration, where the A site usually comprises alkaline- or rare-earth metal elements (Group I or II) whilst the B site consists of transition metal elements, usually contribute to excellent properties, such as magnetic, dielectric, optical or electrical properties [1–7]. They have a wide range of usage in sensors [8–10], capacitors [11], microwave resonators [12, 13], magnetic memory components [14], electrode and electrolyte materials for fuel cells [15, 16] and components for solar cells [17–21]. Double perovskite oxides with mixed B cations (i.e. $A_2BB'O_6$) were introduced in the solid-state field, with the ordered rock salt-like arrangement of corner-sharing $B$–$O$ and $B'$–$O$ bonds in the crystal structure.

Recently, tellurium-based oxides have attracted the attention of researchers due to their structural features and technological applications in various fields, such as microwave communication systems. The microwave dielectric properties of Te$^{6+}$ double perovskites (i.e. $A_2$MgTeO$_6$ ($A = $ Sr, Ca)) were reported by Dias et al; their $\varepsilon'$ values for Sr$_2$MgTeO$_6$ and Ca$_2$MgTeO$_6$ are 14.31 and 13.23, respectively [22]. Besides, the same authors reported that the Sr$_2$ZnTeO$_6$ compound has a $\varepsilon'$ value of 14.1 [23]. These dielectric results could be associated with the tolerance factor, volume, density, and polarizability aspects.

Recently, the focus has been turned to mixed A cations double perovskites (i.e. $AA'B'B'O_6$) which simultaneously display a layered ordering of A site cations and octahedra ordering of B site cations. $AA'B'B'O_6$ with a 1:1 B site ordering has the potential to be excellent in dielectric [24] or ferroelectricity/paraelectricity aspects [25]. For example, Vilesh et al discussed the dielectric properties of BaBiNaTeO$_6$ and BaLaNaTeO$_6$ which have $\varepsilon'$ values of 39.7 and 18.5 at 1 MHz, respectively. This property is attributed to the high density and large grain size of BaBiNaTeO$_6$ and consequently high $\varepsilon'$ [24]. Meanwhile, the dielectric properties of BaBiLiTeO$_6$ and SrBiLiTeO$_6$ have been studied, and the $\varepsilon'$ value of these compounds is 49.5 and 34.4 at 1 MHz, respectively. The latter has a smaller $\varepsilon'$ value because the strong ionic bond of the Sr compounds in SrBiLiTeO$_6$ has a smaller polarizability intern value [26]. However, no clear relationship exists between the grain size or
densification and the dielectric properties in these works because the small-grain BaBiLiTeO$_6$ can still produce a higher ε' than SrBiLiTeO$_6$. These works indicate that applying two different cations at the A site in tellurium-based AA BB'O$_6$ double perovskites can significantly affect the physical properties of double perovskites.

SrLaLiTeO$_6$ reportedly consists of the perfect 1:1 B site ordering of Te$_6^-$ and Li$^+$ that is similar to that in the SrBiLiTeO$_6$ [26] and has an optical band gap of 4 eV [27]. This finding suggests that SrLaLiTeO$_6$ has potential in dielectric or ferroelectricity properties too. To the best of our knowledge, no report about dielectric and conductivity properties of pristine or doped SrLaLiTeO$_6$ can be found in the literature. Investigating the effects of small size Nd doping at the A site in SrLaLiTeO$_6$ on its grain size, dielectric and optical properties is an interesting endeavor. Hence, we report structural, optical, dielectric and conductivity studies on SrNd$_x$La$_{1-x}$LiTeO$_6$ ($x = 0.00, 0.25, 0.50, 0.75, 1.00$).

2. Experimental

Polycrystalline powders of SrLa$_{1-x}$Nd$_x$LiTeO$_6$ ($x = 0.00, 0.25, 0.50, 0.75, 1.00$) were synthesised using the solid-state reaction method. High-purity ($\geq 99.99\%$) strontium carbonate (SrCO$_3$), lithium carbonate (Li$_2$CO$_3$), lanthanum oxide (La$_2$O$_3$), neodymium oxide (Nd$_2$O$_3$) and tellurium dioxide (TeO$_2$) powders were used as raw materials. The chemical powders were mixed at stoichiometric ratios with a total mass of 3 g. The samples were then ground in an agate mortar with a pestle for 1 h to achieve good homogeneity. After grinding, the mixed powder sample was then pressed into a pellet at a pressure of 4–5 kPa using a hydraulic press. The pellet was then placed on an alumina crucible and calcinated in a box furnace at 850 °C for 10 h at a heating rate of 15 °C min$^{-1}$ and a cooling rate of 1 °C min$^{-1}$. Then, the samples were sintered in air at 900 °C for 10 h, followed by slow cooling at 1 °C min$^{-1}$. This action is expected to maintain the obtained stoichiometry near the desired oxygen stoichiometry [28, 29].

The phase(s) of the final products were analyzed using the XRD patterns collected by an x-ray powder diffractometer (PANanalytical model Xpert PRO MPD diffractometer) equipped with a Cu Kα source from 10° to 90°. A General Structure Analysis System and a Graphical User Interface (i.e. EXPGUI) programs [30, 31] were used for Rietveld refinement [32] prior to the visualization in the Visualisation for Electronic Structural Analysis program. The peak shape was modeled by the pseudo-Voight function refined with the cell parameter, the scale factor, the zero factor, and the background function. For the Fourier transform infrared (FTIR) study, samples were prepared by thorough mixing with potassium bromide (KBr), and the infrared reflectance spectra ranging from 400 cm$^{-1}$ to 1500 cm$^{-1}$ were recorded using an FTIR–Raman Drift Nicolet 6700 equipment. The surface morphology of the sintered pellets was obtained using a scanning electron microscope (SEM) characterization using LEO model 982 Gemini equipment. The grain size was measured using the ImageJ software. The dielectric and impedance properties at the frequency range of 50 Hz to 1 MHz were collected using a HIOKI 3532–50 LCR Hi Tester connected to a computer with the sandwich geometry of the electrode pellets. The optical study was performed using a Lambda 750, Perkin Elmer, Waltham, USA equipment in the 2 h to 5 h range.

3. Results and discussions

3.1. Structural analysis

Figure 1 shows the XRD data of SrLa$_{1-x}$Nd$_x$LiTeO$_6$ ($x = 0.00, 0.25, 0.50, 0.75, 1.00$) using the Rietveld refinement technique. Compounds of $x = 0.00$ (Nd 1.00) formed in a single-phase whilst compounds of $x = 0.25$ (Nd 0.25), $x = 0.50$ (Nd 0.50), $x = 0.75$ (Nd 0.75) and $x = 1.00$ (Nd 1.00) have small impurity peaks which consist of excess or unreacted Nd$_2$O$_3$ (marked with asterisk). The reliability ($\chi^2$) values obtained for Nd 0.00, Nd 0.25, Nd 0.50, Nd 0.75 and Nd 1.00 are 1.211, 1.545, 2.307, 2.504 and 4.343, respectively. The good agreement between the observed and calculated interplanar spacings ($d$ values) indicates that all these compounds crystallize in the P2$_1$/n monoclinic structure. The refined lattice angles for all compounds are $\alpha = 90^\circ$ and $\gamma = 90^\circ$, whilst those for Nd 0.00, 0.25, 0.50, 0.75 and 1.00 ($\beta$) are 90.03°, 90.12°, 90.06°, 89.92°, and 89.89°, respectively. The refined unit cell volumes ($V$) for each sample are 250.0, 249.3, 249.2, 247.3, and 248.0 Å$^3$, respectively. Thus, the unit cell volume of the crystal structure decreases as the doping increases, except at concentration $x = 1.00$. This result is consistent with the ionic radius of Nd$^{3+}$ (1.27 Å) that is smaller than that of La$^{3+}$ (1.36 Å). The obtained parameters are presented in table 1. Figure 2 shows the octahedral structure from the ab plane that consists of Te$_6^-$ or Li$^+$ (B site cations) that is alternately surrounded by six O$^{2-}$ atoms, whilst the much larger Sr$^{2+}$ and La$^{3+}$ (A site cations) fill the occupancy between these Te(Li)O$_6$ octahedral layers. Sr$^{2+}$ and La$^{3+}$ are located at (0.497, 0.506, 0.253) for Nd 0.00, (0.495, 0.513, 0.252) for Nd 0.25, (0.497, 0.518, 0.251) for Nd 0.50, (0.501, 0.523, 0.252) for Nd 0.75 and (0.500, 0.527, 0.251) for Nd 1.00. Li$^+$ is placed at (0.5, 0, 0) and Te$^{6+}$ at (0, 0.5, 0). The tolerance factor ($\gamma$) is calculated by the following equation [27]:

\[
\gamma = \frac{r_{Te^6} + r_{Li^+} + \frac{1}{2}r_{O^{2-}}}{\sqrt{2}(r_{Sr^{2+}} + r_{La^{3+}})}
\]
where $R_a$ and $R_a'$ represent the radii of the A site cations ($$ \text{Sr}^{2+} \text{ and } \text{La}^{3+} / \text{Nd}^{3+}$$, respectively), $R_b$ and $R_b'$ represent the radii of the B site cations ($$ \text{Li}^{+} \text{ and } \text{Te}^{6+}$$, respectively), and $R_o$ represents the radius of the oxygen anion ($$ \text{O}^{2-}$$). The ideal cubic structure has a $\tau$ of 1. The decrease in $\tau$ is caused by the small ionic size at the A sites. Hence, the crystal structure is distorted by the tilting phenomenon of the B and B' octahedra. To calculate the distortion factor, the ionic radii used for this calculation are as follows: $\text{Sr}^{2+}$ of 1.44 Å ($\text{CN:12}$), $\text{La}^{3+}$ of 1.36 Å ($\text{CN:12}$), $\text{Nd}^{3+}$ of 1.27 Å ($\text{CN:12}$), $\text{Li}^{+}$ of 0.76 Å ($\text{CN:6}$), $\text{Te}^{6+}$ of 0.56 Å ($\text{CN:6}$) and $\text{O}^{2-}$ of 1.40 Å ($\text{CN:6}$) [33]. The calculated values are $\tau = 0.961$ for Nd 0.00, $\tau = 0.957$ for Nd 0.25, $\tau = 0.953$ for Nd 0.50, $\tau = 0.949$ for Nd 0.75 and $\tau = 0.946$ for Nd 1.00. The reduction of these values is understandable as the doping of small size cations ($\text{Nd}^{3+}$) affects the structural distortion and results in a tolerance factor less than 0.961 [27] as in Nd 0.00. The octahedra tilting angle is calculated by using the following equation:

$$ \tau = \frac{R_a + R_a'}{\sqrt{2 \left( \frac{R_b + R_b'}{2} + R_o \right)}} $$

(1)
The bond length of B cations. The bond between Li and O is longer than that between Te and O because of its hexavalent oxidation state. The octahedral tilting angle calculated for all compounds is the same, suggesting that doping at the A site does not affect the B site angle. The octahedra tilt angle in this compound is attributed to the presence of Sr$^{2+}$, La$^{3+}$, and Nd$^{3+}$ atoms at the A sites because the octahedra tilt is needed to optimize the interatomic distance in (Sr/La/Nd–O) bonds. The bond lengths of (Li–O) and (Te–O) are different, suggesting that the octahedral structure distorts and affects the bond length of B cations. The bond between Li and O is longer than that between Te and O because Li$^{+}$ has a larger ionic radius than Te$^{6+}$, and Te–O has a stronger covalent bond than Li–O because of its hexavalent oxidation state. The crystallite size ($D$) is calculated using the following Scherrer equation [35]:

$$D = \frac{K\lambda}{\beta(\theta) \cos \theta}$$

where $K$ represents a constant (0.94), $\lambda$ represents the wavelength of XRD, $\beta$ represents the full width at half maximum, and $\theta$ represents the angle of the most intense peak in XRD. The $D$ values for these compounds are
The increasing trend of crystallite size from 35.58 nm in Nd 0.00 to 41.60 nm in Nd 1.00 indicates that Nd$^{3+}$ substitution results in better crystallization than the unsubstituted compound.

### 3.2. FTIR analysis

Figure 3 shows the infrared patterns of SrLa$_{1-x}$Nd$_x$LiTeO$_6$ (x = 0.00, 0.25, 0.50, 0.75, 1.00) with important peaks in the range of 400 cm$^{-1}$ to 1000 cm$^{-1}$. The presence of peaks between 455–495 cm$^{-1}$ and 509–521 cm$^{-1}$ can be assigned to the antisymmetric stretching vibrations ($\nu_1$) in the Te(Li)O$_6$ octahedra between the (Te–O–Li) bonds, whilst the peaks between 641–711 cm$^{-1}$ and 722–757 cm$^{-1}$ can be assigned to the symmetric stretching vibration ($\nu_2$) of the Te(Li)O$_6$ octahedra between the Te–O–Li bonds [36–38]. No significant changes in intensity for the $\nu_1$ and $\nu_2$ vibrations are observed when more Nd$^{3+}$ doped at the A site, suggesting that Te(Li)O$_6$ octahedra formation is present in all compounds. An observable predominant strong peak exists at 871 cm$^{-1}$ because of the external mode other than Te(Li)O$_6$ octahedra and it becomes clearer with more dopant.
3.3. SEM analysis

Figure 4 exhibits the surface morphological properties of SrLa$_{1-x}$Nd$_x$LiTeO$_6$. The compounds are formed by rough, agglomerated particles but with nearly the same shape distribution. The SEM image of all samples shows that the particles are crowded together and nearly ‘glued’ to each other, especially in Nd 0.75 and Nd 1.00. SrLa$_{1-x}$Nd$_x$LiTeO$_6$ possessed micrometer-sized grains with considerable porosity, and the porosity decreased as doping increased. The compounds’ grain size range was enhanced from 0.7 – 1.2 μm for Nd 0.00 to 0.9 – 2.0 μm for Nd 0.25, 1.1 – 2.0 μm for Nd 0.50 and 0.6 – 1.5 μm for Nd 1.00. The increase in grain size was consistent with the increment in crystallite size. The increase in grain size in SrLa$_{1-x}$Nd$_x$LiTeO$_6$ until Nd 0.50 may be due to the small cationic–size Nd content increased as more dopant added, resulting in the decline of the grain boundaries’ free energy and led to grain size enhancement. The reduction of grain size in Nd 0.75 and Nd 1.00 was probably due to the increasingly dominant Nd phase with small grain size when the Nd content was high. The energy-dispersive x-ray spectroscopy (EDX) results show that all elements in the compounds are present in the samples.

3.4. UV–Vis analysis

The UV-Vis diffuse reflectance measurements for SrLa$_{1-x}$Nd$_x$LiTeO$_6$ were taken at the wavelength range of 200 nm to 800 nm at room temperature, and figure 5(a) displays the obtained spectra as a function of wavelength (λ). Absorption peaks were observed at 300–400, 500–600, and 700–800 nm. From this plot, the peaks’ intensity increased as the value of doping increased from Nd 0.25 to Nd 1.00. Meanwhile, the Nd 0.00 compound showed no peaks. Hence, these peaks may be related to the charge transfer transition between Nd$^{3+}$ and O$^{2-}$ (valence and conduction band) in the lattice structure. Figure 5(b) exhibits the UV-Vis diffuse spectra of SrLa$_{1-x}$Nd$_x$LiTeO$_6$ plotted according to the Kubelka–Munk equation [27]:

$$F(R) = \frac{(1 - R)^2}{2R}$$

where $R$ represents the diffuse reflectance. By taking the intercept of the extrapolations to zero absorption with the photon energy axis, the absorption edge value can be obtained. The bandgap energy values can be calculated by applying the following equation:
where $\lambda$ represents the wavelength of the absorption edge. Meanwhile, figure 5(c) shows the spectra plotted from Tauc’s equation [39–41]:

$$\left[ F(R) \right]^{1/2} = (h\nu - E_{opt})$$

where $h\nu$ represents the energy, and $E_{opt}$ represents the optical gap energy. In this plot, the values of $E_g$ can be directly obtained by extrapolation without further calculation as shown in figure 5(b). From the Tauc equation, $n$ can be varied from $n = 1/2$ (direct allowed transition), $n = 2$ (indirect allowed transition), $n = 3/2$ (direct forbidden transition) and $n = 3$ (an indirect forbidden transition). The fitting of all the values of $n$ in the Tauc relation indicates that $n = 1/2$ is the most well-fitted. Thus, the optical band gap in this compound has allowed the direct shift of electrons from the valence band to the conduction band where only the absorption of photon occurred because its crystal momentum at both bands was the same. The values of $E_g$ obtained from the Kubelka–Munk and Tauc plots are tabulated in table 2. The values from both methods are comparable to each other. These results are comparable to the reports on the optical properties of SrLaLiTeO$_6$ by Lal et al [42]. The bandgap deformation potential for a physical response to a hydrostatic volume change is given by:

$$E_g = \frac{1240}{\lambda}$$

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Dielectric loss 

\[ \varepsilon' \] shows the variation for SrLa1-xNd_xLiTeO_6 with selected frequencies for different Nd concentration and (b) Tan \( \delta \) of SrLa1-xNd_xLiTeO_6 (x = 0.00, 0.25, 0.50, 0.75, 1.00) within 50–1 MHz.

\[ \alpha_v = \frac{\partial E_g}{\delta \ln V} \]  

where \( V \) is the unit cell volume \[ 43, 44 \]. Therefore, the optical band gap should decrease with the increasing dopant concentration if the deformation is positive. In this work, the optical band gap of the samples decreased as Nd concentration increased till \( x = 0.50 \) which is consistent with the unit cell volume trend. The increase of the bandgap with further doping may be attributed to the increase of the unit cell volume.

Furthermore, the smallest optical band gap was obtained in Nd 0.50, indicating the best conducting ability. This property may due to the presence of polarons in these samples that contribute to conducting ability. The production of polarons in SrLa1-xNd_xLiTeO_6 can be related to the single/double ionized oxygen vacancies formation and most probably caused by the lithium evaporation during high-temperature sintering as suggested by Kroger and Vink \[ 45 \] with the following reaction:

\[ O_2 \rightarrow \frac{1}{2} O_2 + V'_o + 2e^{-1} \]  

where \( V'_o \) represents double ionized oxygen vacancies. Oxygen vacancies contributed to the results in this work. However, the monoclinic structure and the lattice parameters of all samples are comparable to the stoichiometric SrLaLiTeO_6 according to a previous report \[ 27 \]. Hence, the differences in oxygen content amongst the samples are small and should not have a major influence on the measured properties.

Materials with a wide bandgap that can emit light have helped fuel the development of semiconductors in recent years for optoelectronics applications, such as blue/green lasers or light-emitting diode (LED) \[ 46 \]. The high values of the optical band gap obtained are comparable with those in the GaN solid-state (3.5 eV and above) which are usually used as a basis in solid-state LED production to provide an energy-saving, durable, and long-life alternative to incandescent bulbs \[ 47, 48 \].

### 3.5. EIS Dielectric Analysis

The real component of dielectric constant (\( \varepsilon' \)) indicates the ability of the electrical dipoles in the samples to align with the external electric field. Figure 6(a) shows the variation of \( \varepsilon' \) versus frequency between 50 Hz to 1 MHz for the SrLa1-xNd_xLiTeO_6 (x = 0.00, 0.25, 0.50, 0.75, 1.00) samples at 298 K. The specific response of \( \varepsilon' \) towards frequency is different for each sample according to the concentration of the Nd dopant. For frequencies below 100 Hz, the samples showed a nearly similar response of \( \varepsilon' \) variation with the frequency where \( \varepsilon' \) dropped abruptly with the frequency from a higher initial value. However, the specific response for each sample was different at frequencies higher than 100 Hz. For sample Nd 0.00, the response showed a weak decrease in \( \varepsilon' \) with the frequencies. Increasing the Nd dopant in samples Nd 0.25, Nd 0.75, and Nd 1.00 caused a sharper decrease of \( \varepsilon' \) up to 1 MHz. However, for sample Nd 0.50, the \( \varepsilon' \) value was surprisingly, nearly constant at above 100 Hz.

Figure 6(a) (inset) shows the variation of \( \varepsilon' \) at frequencies of 250, 500 and 750 kHz, and the grain size for each Nd concentration was \( x = 0.00, 0.25, 0.50, 0.75, 1.00 \). Interestingly, this variation showed an increasing \( \varepsilon' \) trend up to a peak value in Nd 0.50 before decreasing with a further increase in Nd dopant. This \( \varepsilon' \) maxima apparently coincided with the grain size peak in Nd 0.50.

Figure 6(b) shows the Tan \( \delta \) variation for SrLa1-xNd_xLiTeO_6 (x = 0.00, 0.25, 0.50, 0.75, 1.00) at 298 K. Dielectric loss (Tan \( \delta \)) represents the energy loss during the alternation of electric field onto the samples. This figure shows the drop of Tan \( \delta \) at low frequencies (<500 Hz), followed by a relatively flat trend at intermediate frequencies (600–10 kHz). For samples Nd 0.00 and 0.50, the loss slightly increased at 100 kHz and above.
However, for samples, Nd 0.25, Nd 0.75, and Nd 1.00, a large increase in $\tan \delta$ at the same frequency range can be observed. This indicates the possibility of the presence of a relaxation peak at frequencies higher than 1 MHz.

The initial drop of $\varepsilon'$ at low frequencies ($< 100$ Hz) for all samples in figure 6(a) can be attributed to the heavy dipoles which mainly consist of space charge dipoles. The space charge dipoles were probably due to the defects in grain boundaries that cannot follow the alternation of the electric field as the frequencies increased. This drop was supported by the high value of $\tan \delta$ at the same frequency range in all samples which indicates loss of energy took place. At this frequency range ($< 100$ Hz), the Nd dopant did not seem to significantly affect the heavy space charge dipoles’ contribution to the total polarisation. The defect in the crystal structure, i.e., oxygen vacancies formation, maybe the other reason for the presence of the heavy dipoles in this frequency range. The presence of oxygen vacancies in the insulating compounds can reduce the phonon modes, causing space charge polarization [49]. This drop may also be due to the DC conduction loss. However, the plot of $\ln \varepsilon'$ versus $ln \omega$ does not show a slope of magnitude near ($-1$) to prove the presence of DC conduction loss.

At higher frequencies ($>100$ Hz), the $\varepsilon'$ response was most probably due to the combination of medium- and light-sized dipoles which consist of orientational, ionic, and electronic dipoles. For sample Nd 0.00, the decline of $\varepsilon'$ was correlated with the increase of $\tan \delta$ which can be seen at frequencies higher than 10 kHz. The effect of Nd dopant can be seen at frequencies ranging from 100 kHz to 1 MHz where, for samples Nd 0.25, Nd 0.75 and Nd 1.00, increasing the Nd dopant caused a sharper decrease in $\varepsilon'$ which was related to the larger increase in $\tan \delta$ for frequencies higher than 100 kHz. Above 100 kHz, the medium-sized dipoles in Nd 0.25, NO.75, and Nd 1.00 were not able to follow the external electric field efficiently till 1 MHz, thus producing a low polarisation effect. However, the almost constant $\varepsilon'$ for Nd 0.50 was intriguing but can be related to the nearly constant $\tan \delta$ for the same sample. The absence of a similar increase in $\tan \delta$ with frequency for this sample indicates the abundance of medium-sized dipoles that can respond to high frequencies and produce a higher polarisation value.

The variation of $\varepsilon'$ can be understood better by considering the $\varepsilon'$ trend in the inset of figure 6(a) which is consistent with the grain size trend with the increasing Nd concentration. Larger grains allow the formation of larger medium-sized dipoles with a higher $\varepsilon'$ than smaller grains. In addition, larger grains are expected to carry a higher density of medium-sized dipoles than smaller grains. This phenomenon explains the consistency of the variation in grain size with that of $\varepsilon'$. A similar explanation of the effect of grain size on $\varepsilon'$ is reported in the literature, where $\varepsilon'$ is linearly related to the grain size [50].

Figure 7 illustrates the variation of the $\varepsilon'$ value for SrLa$_{1-x}$Nd$_x$LiTeO$_6$ as a function of temperature in the range of 298 K to 343 K. The $\varepsilon'$ response variation pattern is nearly the same in all samples. All samples showed decrease trend of $\varepsilon'$ at low frequencies until 300 Hz, starting from room temperature to 323 K, except for Nd 0.25 which starting from room temperature to 333 K and for Nd 1.00 which starting from room temperature to 313 K. However, the values exhibit an increasing $\varepsilon'$ pattern at the same frequencies of higher temperatures. Meanwhile, the $\varepsilon'$ value at the intermediate and high frequencies presents a decreasing trend for all temperatures, and the $\varepsilon'$ value increases with the temperature, especially at high frequencies.

Figure 8 illustrates the variation of $\varepsilon'$ with the function of temperature for the Nd 0.50 sample at different frequencies. At frequencies higher than 100 Hz, the plot dispersion was clearly towards higher temperatures. This result shows that $\varepsilon'$ was strongly dependent on frequencies at high temperatures. At most frequencies, the values of $\varepsilon'$ were not increasing linearly with the increasing temperature. The $\varepsilon'$ values decreased at a certain temperature for each frequency. At 100 Hz, the decrease of $\varepsilon'$ started at 303 K. At higher frequencies, the decrease of $\varepsilon'$ shifted towards higher temperatures, except at 1 MHz where the $\varepsilon'$ values increased with the temperature up until 343 K. At 1 MHz, the value of $\varepsilon'$ may decrease at much higher temperatures, following the trend of $\varepsilon'$ at lower frequencies.

Figure 9 illustrates the variation of the $\tan \delta$ of all samples with respect to various temperatures. Two maxima existed at low and higher frequencies. As the temperature increased, the low frequencies maxima were enhanced, whilst the high frequencies maxima were reduced. Nonetheless, in most compounds, no low-frequency maxima existed at the temperature of 333 K and above. This phenomenon can be correlated to the trend at low frequencies in the graph of the $\varepsilon'$ response in figure 7 and most probably pertains to the resonance that occurred in all the samples.

Overall, the declining trend in figure 7 indicates the reduction of the contribution of the heavy space charge when the frequencies increased. However, starting at 333 K (343 K in Nd 0.25 and 323 K in Nd 1.00), the increasing trend of $\varepsilon'$ values at frequencies below 400 kHz can be observed in compounds which is contrary to the declining trend of $\varepsilon'$ values at low temperatures. This finding is most probably due to the dielectric resonant [51]. At high frequencies, the strong temperature dependence of the $\varepsilon'$ value suggests there is more thermal energy to weaken structural bonds and converted into kinetic energy to move the space charge and orientational dipoles to follow electric field alteration as temperature increased. These results suggest two possible effects of high temperature (323 K and above) on the studied samples. One is the weakening of the dipole formations at low frequencies due to the
dielectric resonant. The other is the provision of kinetic energy and weakening structural bonds. Hence, the dipoles’ movement at higher frequencies is facilitated.

Figure 8 shows the weak temperature dependence of the $\varepsilon'$ value at low frequencies, i.e. below 1000 Hz, indicates that dielectric resonant occurred and hindered the dipoles from following the electric field alternation. As the frequency increased, the shifting of $\varepsilon'$ peak towards higher temperatures indicates the effects of temperature in enhancing $\varepsilon'$ values by allowing more thermal energy conversion into kinetic energy to aid dipole movements, before resonant occur at higher temperatures. The largest increase rate of $\varepsilon'$ against temperature is at 1 MHz, indicating the most delocalization of dipoles which consist of orientational and lighter dipoles.

Figure 9 shows that the presence of maxima at low frequencies can be due to the DC conduction loss as discussed earlier. The presence of maxima can also be related to the movement of charge carriers through the grain boundaries. Given the higher resistance of grain boundaries than that of the grain, more energy is required for the motion of carriers through the grain boundaries. Hence, the energy loss is high. For temperatures 333 K and 343 K (including 323 K in Nd 0.75 and Nd 1.00), the shape of the $\tan \delta$ curve is most probably related to the dielectric resonant. Meanwhile, the presence of high-frequency maxima indicates the presence of relaxation.
peaks at high frequencies. Furthermore, the plot indicates possibilities of peaks shifting towards higher frequencies with respect to temperature. This possibility can indicate the results of bond weakening and hence more free movement of dipoles which is more dominant at higher temperatures. Furthermore, this result can also be due to the scattering of thermally induced charge carriers [52].

Figure 10 shows the imaginary modulus plot which is important for determining the charge carrier’s mechanism or relaxation times within the studied compound. However, figure 10 shows no definitive relaxation peaks of SrLa1-xNdxF406. A higher frequency is probably required to determine the relaxation peaks. The plot exhibits a long tail at lower frequencies, specifically at higher temperatures. As the temperature elevated, the presence of long-tail suggests that more delocalization of charge carriers occurred. This is understandable as by conservation of energy, more thermal energy supplied converted into more kinetic energy to embark on the movement of carriers. However, the tails do not start from zero values, indicating the electrode effect of space charge.

The impedance spectroscopy method is widely used to characterize the electrical properties of materials and provide data regarding both the resistive (real) and reactive (imaginary part) components with various transport mechanisms operating within the structure of the material. Figure 11(a) shows the Nyquist plots of the SrLa1-xNdxLiTeO6 compounds. The Low-frequency region consists of the grain boundary resistance, Rgb [53]. The plots of all compounds are straight lines, indicating their high insulating or resistive nature. Nd 0.50 clearly shows the largest Rgb whilst Nd 0.00 shows the smallest Rgb with 1.3 × 106 Ω and 4.6 × 106 Ω, respectively, which are consistent with their ε’ trend. The fitted semi-circular arcs show a slight distortion, indicating the deviation from the Debye mechanism. Figure 11(b) displays the variation of DC conductivity of SrLa1-xNd0.50LiTeO6 compounds against temperatures. These plots have R2 values ranging from 0.98 to 0.99. To calculate the value of activation energy (Ea) the following Arrhenius’ equation applied:

$$\sigma_{DC} = \sigma_0 e^{-E_a/kT}$$

where $k_B$ represents the Boltzmann constant. The calculated Ea for Nd 0.00, Nd 0.25, Nd 0.50, Nd 0.75 and Nd 1.00 are 0.0596, 0.0620, 0.0622, 0.0609 and 0.0599 eV, respectively.

To calculate the capacitance of SrLa1-xNd0.50LiTeO6, the following equation is used:

$$C = \varepsilon_0 \varepsilon' (A/d)$$

where $\varepsilon_0$ represents the vacuum permittivity, $A$ represents the area of contact between compounds and electrode whilst $d$ represents the thickness of compounds. The calculated capacitance values at room temperature at 1 MHz for Nd 0.00, Nd 0.25, Nd 0.50, Nd 0.75, and Nd 1.00 are 3.5025 pF, 7.83324 pF, 20.6073 pF, 7.88707 pF, and 4.93076 pF, respectively. These results indicate that Nd 0.50 possesses the most capacitive character among the compounds, consistent with the ε’ trend.

For the AC electrical property, AC conductivity takes place only when the induced electric field present towards the compounds. Figure 12(a) displays the plot of the AC conductivity of Nd 0.50 which displays two distinct regions, a low-frequency dispersive region. The value of $\sigma_{AC}$ increased significantly from a low frequency to 100 kHz. At higher frequencies, a near plateau region existed from 100 kHz to 1 MHz. The variation of conductivity in the low-frequency region was due to the polarisation effects at the electrode and perovskite interfaces. The conductivity decreased as the frequency decreased due to the increased accumulation charge at
the electrode and perovskite interfaces. The conductivity was nearly frequency-independent at higher frequencies (plateau region). The extrapolation of the plateau region on the log $\sigma_{AC}$ provides $\sigma_{DC}$ for SrLa$_{1-x}$Nd$_x$LiTeO$_6$. For Nd 0.50, the obtained DC conductivity is determined at $4.4 \times 10^{-9}$ S cm$^{-1}$ at room temperature. Meanwhile, $\sigma_{AC}$ may exhibit a higher value of $\sigma_{AC}$ at higher frequencies to show the same trend of $\sigma_{AC}$ as in other ceramic double perovskites [53, 55]. This is correlated with the probability of peaks at higher frequencies in the plot of $\varepsilon'$ and $\tan \delta$ as previously discussed. Hence, the AC conductivity of SrLa$_{1-x}$Nd$_x$LiTeO$_6$ can be related to Jonscher’s power law [56]:

$$\sigma_T = \sigma_{DC} + A\omega^s$$

where $A$ represents pre-exponential constant, $\omega = 2\pi f$ represents the angular frequency and $s$ represents power-law exponent, where $0 < s < 1$. From this equation, $\sigma_{DC}$ is the DC conductivity whereas $A\omega^s$ is the AC conductivity.

The plot of $\ln \varepsilon'$ against $\ln \omega$ (not shown) indicates that the value of $s$ obtained is less than 1. According to Funke [55], when $s < 1$ charge carriers in compounds take a translational motion with a sudden hopping between sites in the lattice whilst when $s > 1$, localized hopping can occur in the lattice sites. Hence, the

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Figure 9. $\tan \delta$ of SrLa$_{1-x}$Nd$_x$LiTeO$_6$ ($x = (a) 0.00, (b) 0.25, (c) 0.50, (d) 0.75 and (e) 1.00$) at different temperatures.
calculated $s$ value indicates that the charge carriers in SrLa$_{1-x}$Nd$_x$LiTeO$_6$ can move over a long-range with translational motion. The charge carriers involved in SrLa$_{1-x}$Nd$_x$LiTeO$_6$ are most probably polarons that formed with the occurrence of oxygen vacancies.

Figure 10. $M''$ of Nd 0.50 at different temperatures.

Figure 11. (a) Impedance of SrLa$_{1-x}$Nd$_x$LiTeO$_6$ ($x = 0.00, 0.25, 0.50, 0.75, 1.00$) at room temperature and (b) Variation of dc conductivity of SrLa$_{1-x}$Nd$_x$LiTeO$_6$ with temperatures.

Figure 12. (a) $\sigma_{AC}$ Nd 0.50 and (b) variation of $s$ with temperatures for SrLa$_{1-x}$Nd$_x$LiTeO$_6$. 
To further confirm the AC conduction mechanism in SrLa\(_{1-x}\)Nd\(_x\)LiTeO\(_6\), the variation of \(s\) with different temperatures is plotted. Figure 12(b) shows the variation of \(s\) with different temperatures. This figure indicates that the variation of \(s\) decreases until the temperature of 323 K and increases again until the temperature of 343 K. Some mechanisms of AC conductivity have been suggested by researchers in previous studies, i.e. correlated barrier hopping [57, 58], variable range hopping [59], small polaron hopping [60, 61], quantum mechanical tunneling [62], non-overlapping small polaron tunneling [63] and overlapping large polaron tunneling (OLPT) [64]. Figure 12(c) shows that the most suitable model for all compounds is the OLPT mechanism model that exhibits a decreasing trend of \(s\) values with the temperature before starting to increase at a certain temperature which is the same trend reported for other ceramics [65]. The AC conductivity for the overlapping large polaron tunneling model is expressed as:

\[
\sigma' (\omega) = \frac{\pi^2 e^2 (k_B T)^2 [N (E_F)]^2 \omega R_w^4}{12 \alpha k_B T + \frac{8\eta N_{\text{ho}}}{R_w^2}}
\]

(12)

where \(\alpha\) represents the decay parameter for the localized wave function, \(N (E_F)\) represents the density of the localized state, \(k_B\) represents Boltzmann’s constant, \(T\) represents the absolute temperature, \(W_{\text{ho}}\) represents the activation energy associated with the charge transfer between overlapping sites, \(r_p\) represents the polaron radius and \(R_w\) represents the tunneling length at frequency \(\omega\). For the frequency exponent, the \(s\) predicted by this model is expressed as follows [66]:

\[
s = 1 - \frac{8\alpha R_w + 6W_{\text{ho}}r_p/R_w k_B T}{[(2\alpha R_w + W_{\text{ho}}r_p)/R_w k_B T]^2}
\]

(13)

The polarons can tunnel between two or more sites in the lattice structure with more or less hopping movement between defects or energy wells. The large polaron is the excitation due to the polaron tunneling in the deformed lattice in which the change of the polarisation yields the polaron energy. In the case of the OLPT, the large polaron wells overlap at two sites by reducing the polaron hopping energy [65]. Henceforth, this mechanism can be related to the small value activation energy of polarons as calculated using equation (9).

4. Conclusion

SrLa\(_{1-x}\)Nd\(_x\)LiTeO\(_6\) (\(x = 0.00, 0.25, 0.50, 0.75, 1.00\)) compounds were prepared using the solid-state reaction method and crystallised into a \(P2_1/n\) primitive monoclinic structure. The IR spectra exhibit the characteristic bands of Te(Li)O bonds, confirming the ‘fingerprint’ structure of this double perovskite. The SEM images reveal that grain size increases when dopant is added up until \(x = 0.50\), whilst the grain size in the compound with \(x = 0.75\) and \(x = 1.00\) decreases. The UV-Vis study reports the decrease of \(E_{\text{opt}}\) as the doping increases from Nd 0.00 to Nd 0.50. The frequency and temperature dependence of the real permittivity and DC conductivity of SrNd\(_{0.5}\)La\(_{0.5}\)LiTeO\(_6\) were characterized by impedance spectroscopy. Nd 0.50 recorded the highest \(\varepsilon'\) value of 165 at room temperature. This behavior explained on the basis of grain size enhancement. To further enhance the \(\varepsilon'\) value, the sintering parameters can be altered to increase the densification as in the other reports. Meanwhile, the AC conductivity plot follows the universal power law, and the nature of AC conductivity can be explained using the OLPT model with polarons as charge carriers.

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