**Supporting Information**

**Synthesis and lithium-ion conductivity of Sr(La1−*x*Li3*x*)ScO4 with a K2NiF4 structure**

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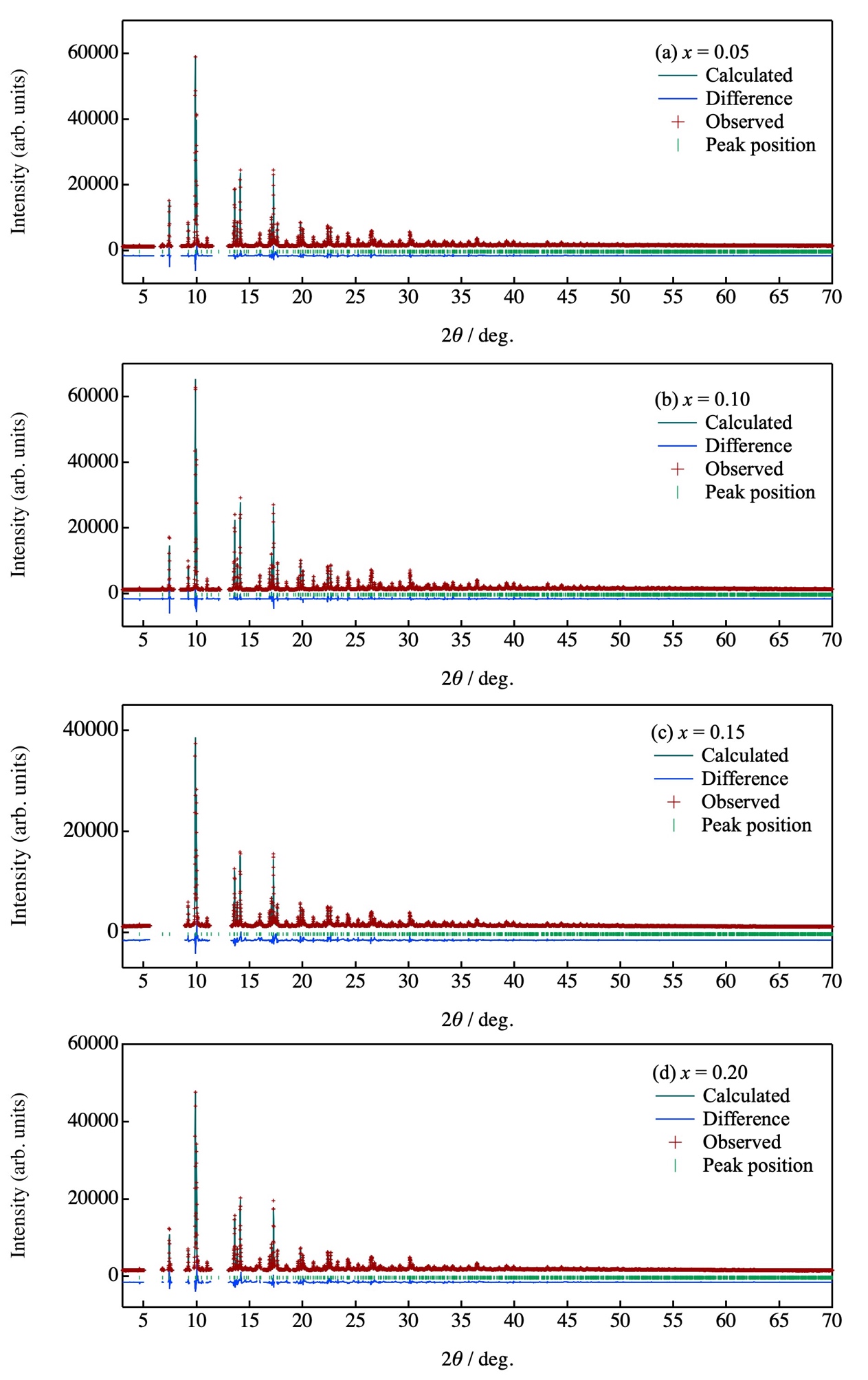
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**Figure. S1.** Synchrotron powder diffraction and Rietveld refinement patterns for Sr(La1−*x*Li3*x*)ScO4 (*x* = 0.05, 0.10, 0.15 and 0.20) at 300 K: (a) *x* = 0.05, (b) *x* = 0.10,(c) *x* = 0.15, and (d) *x* = 0.20. Red: observed intensities; Black: calculated intensities; blue: difference plot. The green markers indicate the positions of the diffraction lines.

**Table S1.** Results obtained from the Rietveld refinement of the synchrotron X-ray diffraction pattern of Sr(La1−*x*Li3*x*)ScO4.a

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Atom** | **Site** | ***g***b | | ***x*** | ***y*** | | ***z*** | ***B*iso (**Å2)c |
| (1) *x* = 0.05, SrLa0.95Li0.15ScO4, space group: *Abma* (No. 64), *a* = 5.7654(15) Å, *b* = 5.7574(13) Å, *c* = 12.4825(2) Å, *V* = 414.41(16) Å3, *R*wp = 6.018, *R*p = 3.271, *R*e = 2.313, *S* = *R*wp/*R*e = 2.602, *R*f = 1.229 | | | | | | | | |
| Li1/Li | 8*f* | 0.025 | | =*x*(La) | | =*y*(La) | =*z*(La) | =*B*iso. (La) |
| Sr | 8*f* | 0.5 | | =*x*(La) | | =*y*(La) | =*z*(La) | =*B*iso. (La) |
| La | 8*f* | 0.475 | | 0.0140(3) | | 0 | 0.35674(6) | 0.57(2) |
| Sc | 4*a* | 1.0 | | 0 | | 0 | 0 | 0.58(5) |
| O1 | 8*e* | 1.0 | | 0.25 | | 0.25 | 0.0183(8) | 2.0(2) |
| O2 | 8*d* | 1.0 | 0.437(17) | | | 0 | 0.3268(5) | 0.7(2) |
| (2) *x* = 0.10, SrLa0.90Li0.30ScO4, space group: *Abma* (No. 64), *a* = 5.76376(8) Å, *b* = 5.75654(8) Å, *c* = 12.4725(13) Å, *V* = 413.829(9) Å3, *R*wp = 5.156, *R*p = 2.970, *R*e = 2.370, *S* = *R*wp/*R*e = 2.175, *R*f = 1.317 | | | | | | | | |
| Li1/Li | 8*f* | 0.05 | =*x*(La) | | | =*y*(La) | =*z*(La) | =*B*iso. (La) |
| Sr | 8*f* | 0.5 | =*x*(La) | | | =*y*(La) | =*z*(La) | =*B*iso. (La) |
| La | 8*f* | 0.45 | 0.0129(19) | | | 0 | 0.35701(5) | 0.38(15) |
| Sc | 4*a* | 1.0 | 0 | | | 0 | 0 | 0.69(4) |
| O1 | 8*e* | 1.0 | 0.25 | | | 0.25 | 0.0167(6) | 1.0(13) |
| O2 | 8*d* | 1.0 | 0.438(13) | | | 0 | 0.3297(4) | 1.5(2) |
| (3) *x* = 0.15, SrLa0.85Li0.45ScO4, space group: *Abma* (No. 64); *a* = 5.7681(14) Å, *b* = 5.7602(12) Å, *c* = 12.4913(17) Å, *V* = 415.03(14) Å3, *R*wp = 6.642, *R*p = 3.785, *R*e = 2.582, *S* = *R*wp/*R*e = 2.572, *R*f = 2.703 | | | | | | | | |
| Li1/Li | 8*f* | 0.075 | =*x*(La) | | | =*y*(La) | =*z*(La) | =*B*iso. (La) |
| Sr | 8*f* | 0.5 | =*x*(La) | | | =*y*(La) | =*z*(La) | =*B*iso. (La) |
| La | 8*f* | 0.425 | 0.0141(4) | | | 0 | 0.35681(8) | 0.61(2) |
| Sc | 4*a* | 1.0 | 0 | | | 0 | 0 | 1.04(7) |
| O1 | 8*e* | 1.0 | 0.25 | | | 0.25 | 0.021(12) | 3.1(3) |
| O2 | 8*d* | 1.0 | 0.443(3) | | | 0 | 0.3248(7) | 0.7(2) |
| (4) *x* = 0.20, SrLa0.80Li0.60ScO4, space group: *Abma* (No. 64), *a* = 5.7655(2) Å, *b* = 5.7569(19) Å, *c* = 12.4837(3) Å, *V* = 414.36(2) Å3, *R*wp = 6.510, *R*p = 3.518, *R*e = 2.246, *S* = *R*wp/*R*e = 2.899, *R*f = 1.555 | | | | | | | | |
| Li1/Li | 8*f* | 0.1 | =*x*(La) | | | =*y*(La) | =*z*(La) | =*B*iso. (La) |
| Sr | 8*f* | 0.5 | =*x*(La) | | | =*y*(La) | =*z*(La) | =*B*iso. (La) |
| La | 8*f* | 0.4 | 0.0137(4) | | | 0 | 0.35681(8) | 0.63(3) |
| Sc | 4*a* | 1.0 | 0 | | | 0 | 0 | 1.34(7) |
| O1 | 8*e* | 1.0 | 0.25 | | | 0.25 | 0.020(10) | 2.5(3) |
| O2 | 8*d* | 1.0 | 0.438(2) | | | 0 | 0.3243(6) | 1.4(3) |

aSpace group: *Abma* (64); bsite occupancy, *g*; and cisotropic atomic displacement parameter, *B*iso.

**Table S2.**

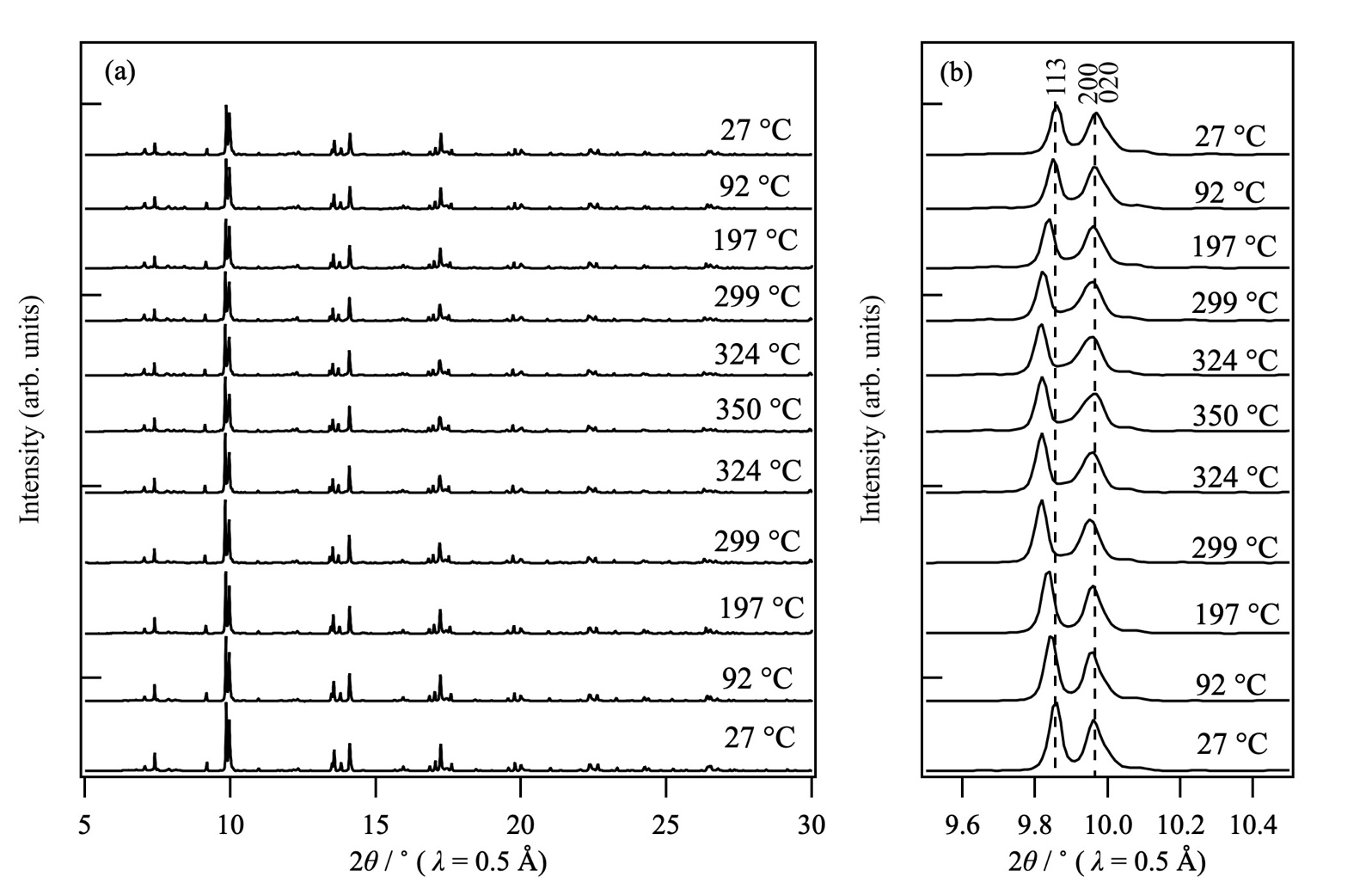
Numerical fitting results of the sample spectra obtained using electrochemical impedance spectroscopy at a representative temperature of 250 ℃. Chi-square is an ideality factor used to evaluate the goodness of the fit.

|  |  |  |
| --- | --- | --- |
| Sample composition | Sr(La0.95Li0.15)ScO4  (*x* = 0.05) | Sr(La0.90Li0.30)ScO4  (*x* = 0.1) |
| Chi square | 0.05 | 0.003 |
| CPE1-T (CPE1, total) | 4.05E−11 | 6.07E−11 |
| CPE1-P (n1, total) | 0.99 | 0.92 |
| R1 (total/Ω) | 3315400 | 1250300 |
| Ws1-R | 3.6E5 | 1.25E6 |
| Ws1-T | 52.26 | 13.15 |
| Ws1-P | 0.84 | 0.63 |
| Thickness (*L*)[cm] | 0.1 | 0.1 |
| Area (*S*)[cm2] | 0.071 | 0.071 |
| Total conductivity (σtotal) [S/cm] | 3.32 × 10−7 | 4.66 × 10−6 |
| **Sample composition** | Sr(La0.85Li0.45)ScO4  (*x* = 0.15) | Sr(La0.8Li0.60)ScO4  (*x* = 0.2) |
| Chi square | 0.003 | 0.013 |
| CPE1-T (CPE1, total) | 1.33E−11 | 7.51E−11 |
| CPE1-P (n1, total) | 0.95 | 0.95 |
| R1 (total/Ω) | 255690 | 956210 |
| Ws1-R | 6.25E6 | 4.36E6 |
| Ws1-T | 52.7 | 22.83 |
| Ws1-P | 0.95 | 0.60 |
| Thickness (*L*)[cm] | 0.09 | 0.11 |
| Area (*S*)[cm2] | 0.075 | 0.075 |
| Total conductivity (σtotal) [S/cm] | 1.13 × 10−6 | 1.52 × 10−6 |

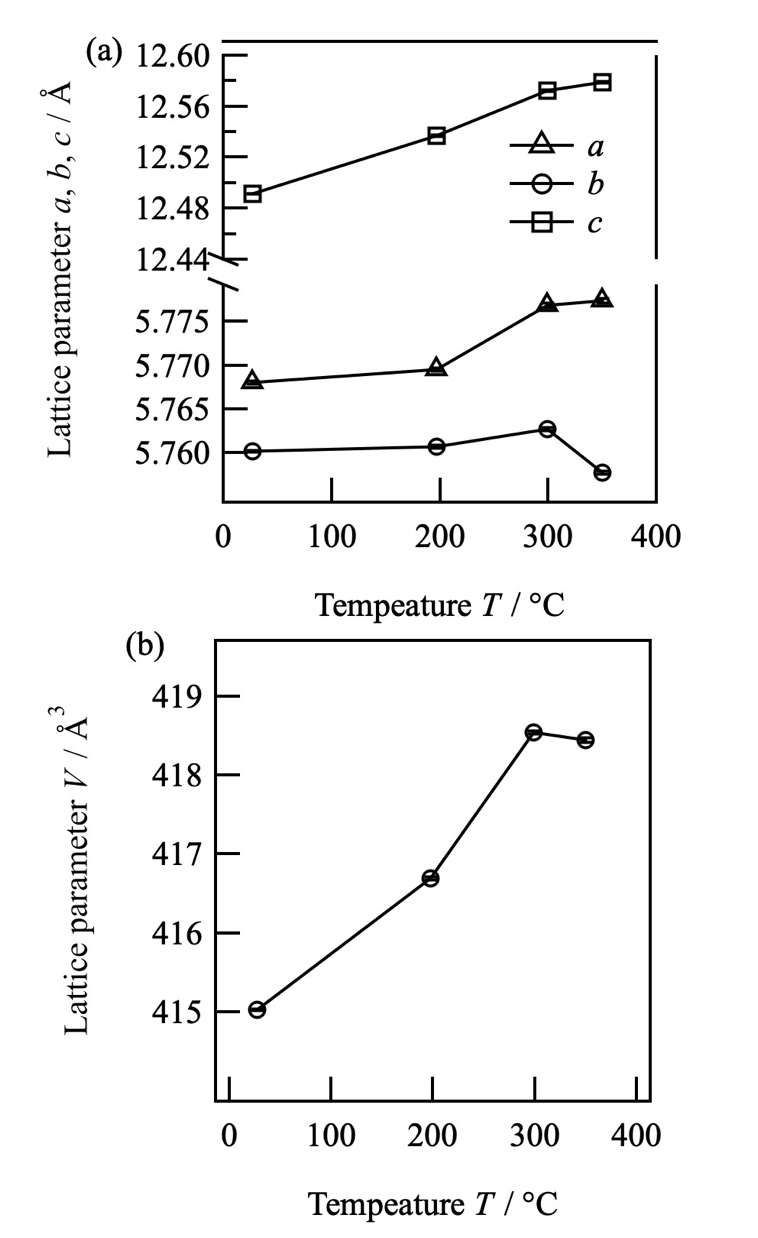
**Table S3.**

Summary of the total conductivity (stotal) measured at different temperatures and the activation energy (*E*a) fitted with the conventional Arrhenius law in the lower-temperature region (<270 °C).

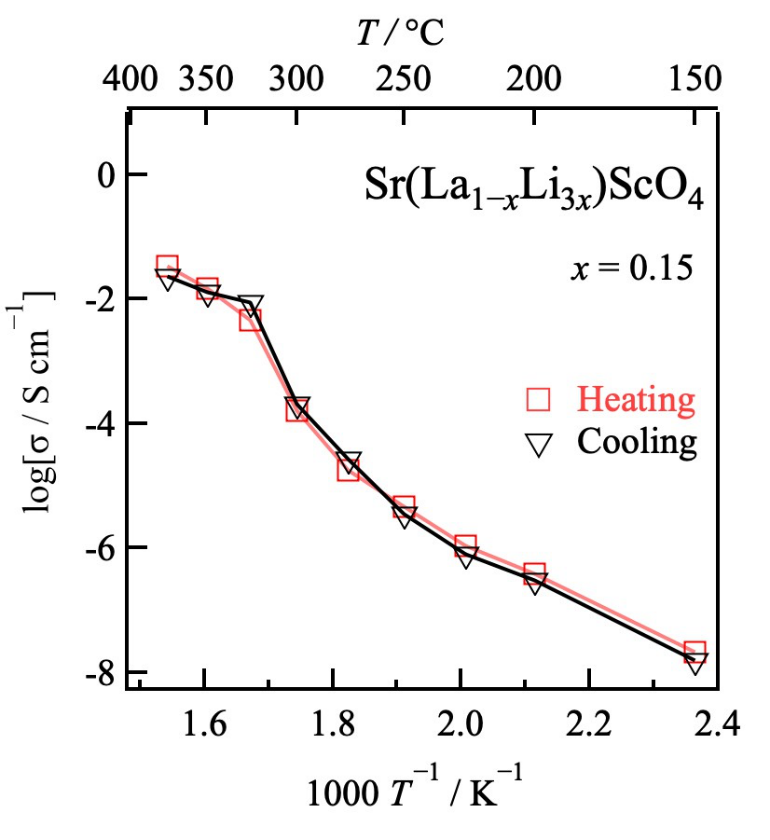
|  |  |  |  |
| --- | --- | --- | --- |
| Temperature  *T* / ℃ | Resistance  *R* / Ω | stotal  / Scm-1 | *E*a  / kJ mol-1 |
| Sr(La0.95Li0.15)ScO4 | | | |
| 210 | 3.31E+07 | 4.00E-08 | 117.6 |
| 250 | 3.32E+06 | 4.00E-07 |
| 275 | 1.01E+06 | 1.31E-06 |
| 310 | 2.01E+05 | 6.60E-06 |
| 350 | 5.64E+03 | 2.35E-04 |
| 375 | 1.08E+03 | 1.22E-03 |
| 400 | 1.27E+02 | 1.04E-02 |
| Sr(La0.90Li0.30)ScO4 | | | |
| 150 | 7.02E+07 | 2.01E-08 | 94.3 |
| 200 | 1.16E+07 | 1.21E-07 |
| 225 | 4.59E+06 | 3.08E-07 |
| 250 | 1.25E+06 | 1.13E-06 |
| 275 | 4.69E+05 | 3.02E-06 |
| 300 | 1.04E+05 | 1.36E-05 |
| 325 | 1.41E+04 | 1.00E-04 |
| 350 | 5.14E+02 | 2.75E-03 |
| 375 | 2.92E+02 | 4.85E-03 |
| 400 | 3.40E+02 | 4.16E-03 |
| Sr(La0.85Li0.45)ScO4 | | | |
| 150 | 5.67E+07 | -17.67781 | 103.4 |
| 200 | 3.04E+06 | -14.75003 |
| 225 | 1.09E+06 | -13.72873 |
| 250 | 2.56E+05 | -12.27574 |
| 275 | 6.71E+04 | -10.93801 |
| 300 | 7.27E+03 | -8.715665 |
| 325 | 2.60E+02 | -5.384697 |
| 350 | 8.00E+01 | -4.206042 |
| 375 | 3.50E+01 | -3.379364 |
| Sr(La0.8Li0.60)ScO4 | | | |
| 200 | 1.97E+07 | 7.40E-08 | 99.3 |
| 250 | 9.56E+05 | 1.52E-06 |
| 275 | 2.92E+05 | 4.98E-06 |
| 300 | 3.30E+04 | 4.42E-05 |
| 325 | 4.35E+02 | 3.35E-03 |
| 350 | 5.30E+01 | 2.75E-02 |
| 375 | 3.40E+01 | 4.29E-02 |



**Figure. S2.** High-temperature X-ray diffraction patterns of Sr(La1−*x*Li3*x*)ScO4 (*x* = 0.15): (a) in 2*θ* range of 5°–30°; (b) in 2*θ* range of 9.6°–10.4°, showing the peaks corresponding to the 113, 200, and 020 reflections. The powder sample was heated to 350 °C, and then cooled to 27 °C. The X-ray diffraction patterns are arranged in the order of heating process and cooling process, from bottom to top.



**Figure. S3.** Temperature dependence of the lattice parameters of Sr(La1−*x*Li3*x*)ScO4 (*x* = 0.15), determined by the Rietveld analysis of the X-ray diffraction data.



**Figure. S4.** Temperature-dependence of the conductivities of Sr(La1−*x*Li3*x*)ScO4 (*x* = 0.15) during heating and cooling processes.