

Supplementary Information for:

Nature of conductivity in SrSiO_3 -based fast ion conductors

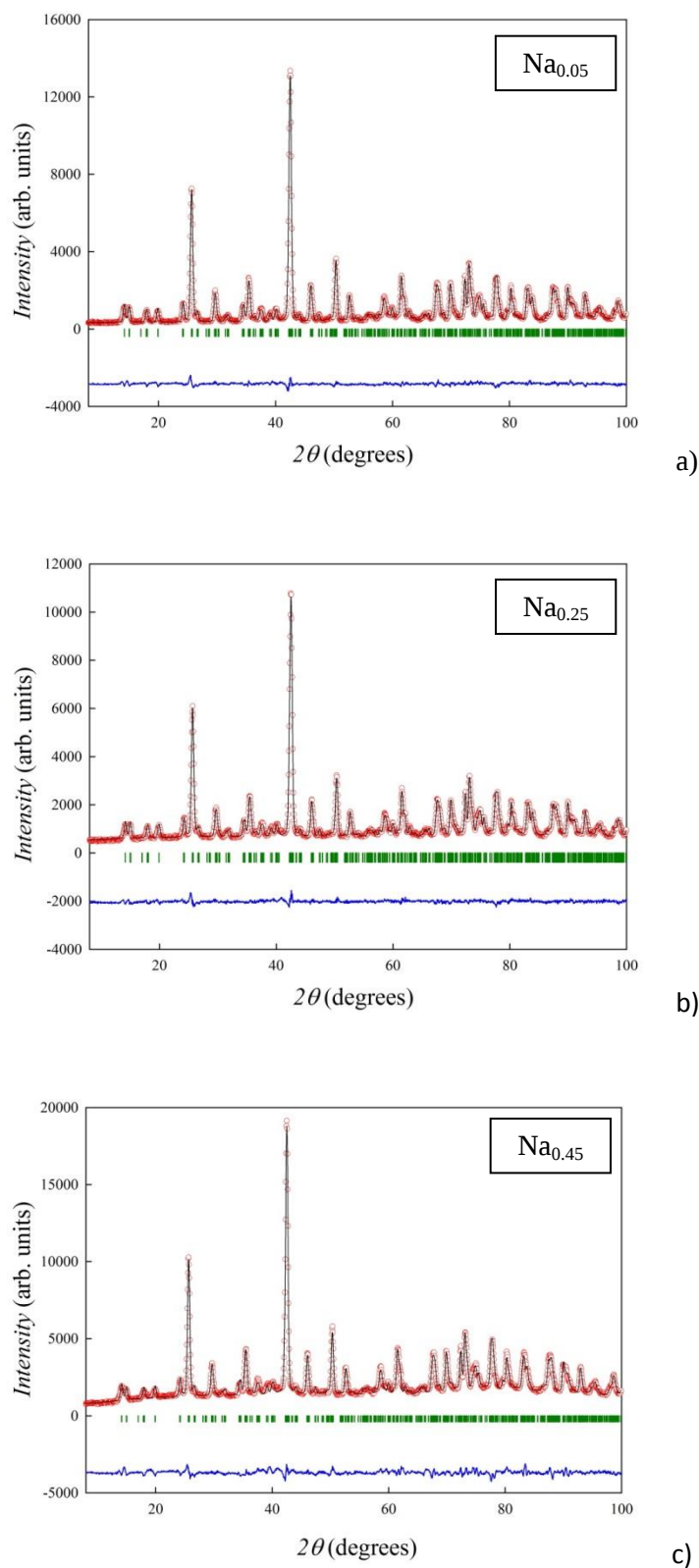


Figure SI-1 Rietveld refined NPD patterns of $\text{Sr}_{1-x}\text{Na}_x\text{SiO}_{3-0.5x}$ showing the experimental (red circle), calculated (black line) and difference profile (blue line). Vertical green lines refer to the theoretical Bragg peaks for SrSiO_3 .

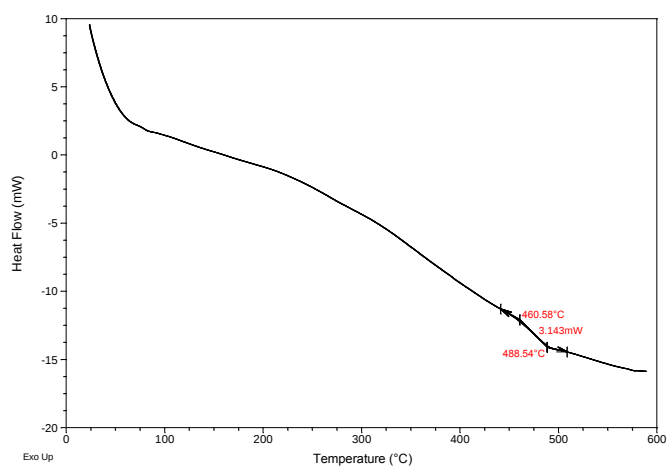


Figure SI-2 DSC scan of the $\text{Na}_{0.45}$ sample indicating the range of the glass phase transition.

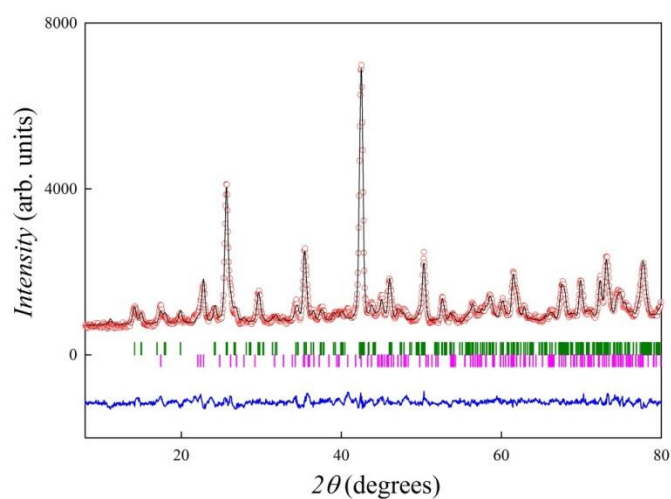


Figure SI-3 Two phases Rietveld refined NPD pattern of the sample of nominal composition $\text{Sr}_{0.55}\text{Na}_{0.45}\text{SiO}_{2.875}$ showing the experimental (red circle), calculated (black line) and difference profile (blue line). Vertical green lines refer to the theoretical Bragg peaks for SrSiO_3 ; vertical pink lines refer to the theoretical Bragg peaks for $\alpha\text{-Na}_2\text{Si}_2\text{O}_5$.

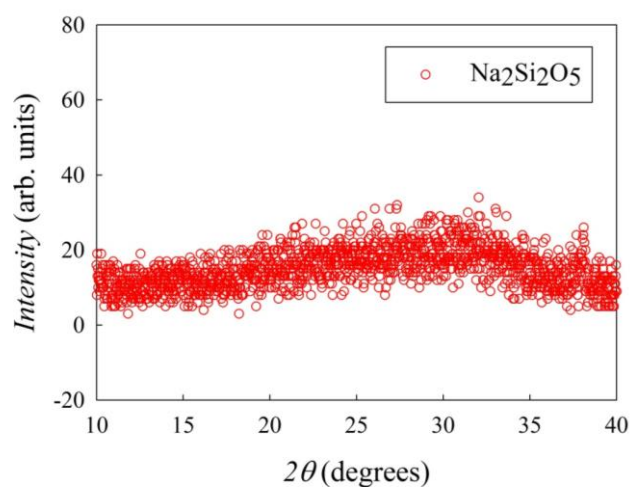


Figure SI-4 Experimental X ray diffraction pattern of the $\text{Na}_2\text{Si}_2\text{O}_5$ phase prepared at 1050°C showing the amorphous nature of the sample. The small pick at $\sim 38^{\circ}$ can be attributed to the Al sample holder.

Table 1 – Rietveld refine structural parameters from NPD data.

Na_{0.05}: R_{wp} - 9.23; R_{Bragg} - 3.60; χ^2 - 2.736Na_{0.25}: R_{wp} - 10.5; R_{Bragg} - 3.60; χ^2 - 2.206Na_{0.45}: R_{wp} - 13.8; R_{Bragg} - 6.52; χ^2 - 5.584

Sample		Na _{0.05}	Na _{0.25}	Na _{0.45}
<i>a</i> (Å)		12.3362 (4)	12.3331 (4)	12.3404 (7)
<i>b</i> (Å)		7.1467 (2)	7.1464 (2)	7.1437 (4)
<i>c</i> (Å)		10.8855 (3)	10.8831 (3)	10.8917 (6)
β (deg)		111.594 (2)	111.584 (2)	111.680 (3)
<i>V</i> (Å ³)		892.35 (4)	891.95 (5)	892.25 (8)
Sr1/Na1	<i>x</i>	0.0870 (3)	0.0870 (3)	0.0873 (5)
	<i>y</i>	0.2420 (4)	0.2416 (4)	0.2447 (7)
	<i>z</i>	0.4997 (4)	0.4995 (5)	0.5006 (8)
	<i>B</i>	0.77 (7)	0.91 (8)	0.80 (5)
Sr2/Na2	<i>x</i>	0.25	0.25	0.25
	<i>y</i>	0.25	0.25	0.25
	<i>z</i>	0	0	0
	<i>B</i>	0.3 (1)	0.5 (1)	0.5 (1)
Si1	<i>x</i>	0.1247 (4)	0.1238 (5)	0.1248 (9)
	<i>y</i>	0.4573 (7)	0.4566 (8)	0.4549 (2)
	<i>z</i>	0.2462 (4)	0.2445 (5)	0.2421 (8)
	<i>B</i>	0.63 (8)	0.64 (9)	0.63 (7)
Si2	<i>x</i>	0	0	0
	<i>y</i>	0.832 (1)	0.832 (1)	0.8272 (2)
	<i>z</i>	0.25	0.25	0.25
	<i>B</i>	1.3 (1)	1.0 (1)	1.1 (1)
O1	<i>x</i>	0.1277 (3)	0.1275 (3)	0.1282 (6)
	<i>y</i>	0.4090 (6)	0.4084 (7)	0.4094 (1)
	<i>z</i>	0.1059 (3)	0.1055 (3)	0.1069 (5)
	<i>B</i>	1.00 (6)	1.02 (7)	1.02 (6)
O2	<i>x</i>	0.2222 (3)	0.2222 (3)	0.2208 (6)
	<i>y</i>	0.4069 (6)	0.4049 (7)	0.4083 (1)
	<i>z</i>	0.3858 (3)	0.3854 (3)	0.3865 (5)
	<i>B</i>	0.79 (6)	0.97 (7)	0.81 (1)
O3	<i>x</i>	0.1067 (3)	0.1073 (3)	0.1090 (7)
	<i>y</i>	0.6890 (5)	0.6900 (5)	0.6880 (1)
	<i>z</i>	0.2478 (3)	0.2483 (4)	0.2480 (2)
	<i>B</i>	0.14 (8)	0.36 (8)	0.22 (6)
O4	<i>x</i>	0.0474 (3)	0.0473 (4)	0.0472 (3)
	<i>y</i>	0.9345 (6)	0.9351 (7)	0.9347 (2)
	<i>z</i>	0.3891 (3)	0.3894 (3)	0.3899 (5)
	<i>B</i>	1.10 (7)	1.05 (8)	1.06 (7)
O5	<i>x</i>	0	0	0
	<i>y</i>	0.3692 (7)	0.3699 (7)	0.3698 (6)
	<i>z</i>	0.25	0.25	0.25
	<i>B</i>	0.67 (1)	0.85 (1)	0.73 (4)