Supporting Information for

Effect of W and Mo co-substituting on conductivity and structure of LaNbO4

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**Figure S1.** Microstructure obtained from the surface (left column) and cross section (right column) of (a), (b) LNMo20; (c),(d) LNW4Mo16; (e),(f) LNW10Mo10; (g), (h) LNW16Mo4; (i), (j) LNW18Mo2.

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**Figure S2.** XRD patterns of LNW2Mo18 recorded around 600 °C. The satellite reflections of the modulated structure are marked by the arrows.

A diagram of a graph

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**Figure S3.** Impedance spectrum of LNMo20 measured at 500 °C. The hollow circles represent the experimental data, and the red line represents the fitting results using the model in the inset.

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**Figure S4.** Conductivities and unit cell volumes of LaNb0.8WxMo0.2-xO4.1 series at around 650 °C, error bars are smaller than the symbols.

**Table S1.** Refined structural parameters of all samples from Rietveld refinements against XRD data collected at 25 °C.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | LNMo20 | LNW2Mo18 | LNW4Mo16 | LNW10Mo10 | LNW16Mo4 | LNW18Mo2 | LNW20 |
| Space group | I 1 2/a 1 | I 1 2/a 1 | I 41/a | I 41/a | I 41/a | I 41/a | I 41/a |
| a (Å) | 5.4001(8) | 5.3995(5) | 5.3487(5) | 5.3402(4) | 5.3348(9) | 5.3352(3) | 5.3361(4) |
| b (Å) | 5.3071(3) | 5.3082(5) | - | - | - | - | - |
| c (Å) | 11.6460(7) | 11.6455(2) | 11.6647(3) | 11.6881(9) | 11.6973(3) | 11.6943(8) | 11.6897(8) |
| β (°) | 91.269(1) | 91.182(2) | - | - | - | - | - |
| V (Å3) | 333.682(9) | 333.711(2) | 333.712(1) | 333.317(2) | 332.904(2) | 332.873(6) | 332.856(9) |
| Rwp (%) | 6.75 | 6.77 | 7.32 | 9.06 | 7.55 | 7.30 | 10.75 |
| χ2 | 7.16 | 4.85 | 5.16 | 4.35 | 4.96 | 4.60 | 7.24 |

**Table S2.** Refined structural parameters of all samples from Rietveld refinements against XRD data collected at 850 °C.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | LNMo20 | LNW2Mo18 | LNW4Mo16 | LNW10Mo10 | LNW16Mo4 | LNW18Mo2 | LNW20 |
| Space group | I 41/a | I 41/a | I 41/a | I 41/a | I 41/a | I 41/a | I 41/a |
| a (Å) | 5.4028(2) | 5.4014(4) | 5.3984(3) | 5.3865(3) | 5.3788(3) | 5.3787(5) | 5.3809(6) |
| c (Å) | 11.7685(4) | 11.7742(6) | 11.7887(4) | 11.8061(4) | 11.8190(5) | 11.8142(6) | 11.8088(9) |
| V (Å3) | 343.526(4) | 343.516(8) | 343.552(8) | 342.544(1) | 341.946(6) | 341.798(9) | 341.914(8) |
| Rwp (%) | 5.25 | 8.10 | 6.28 | 6.02 | 7.45 | 8.41 | 10.64 |
| χ2 | 5.40 | 5.98 | 4.63 | 4.13 | 5.04 | 5.50 | 7.56 |

**Table S3.** Refined structural parameters of all samples from Rietveld refinements against XRD data collected at 650 °C.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | LNMo20 | LNW2Mo18 | LNW4Mo16 | LNW10Mo10 | LNW16Mo4 | LNW18Mo2 | LNW20 |
| Space group | I 41/a | I 41/a | I 41/a | I 41/a | I 41/a | I 41/a | I 41/a |
| a (Å) | 5.3882(3) | 5.3883(3) | 5.3841(3) | 5.3722(3) | 5.3658(3) | 5.3672(3) | 5.3679(5) |
| c (Å) | 11.7385(1) | 11.7416(5) | 11.7577(5) | 11.7776(5) | 11.7877(5) | 11.7857(6) | 11.7792(8) |
| V (Å3) | 340.796(4) | 340.911(5) | 340.839(5) | 339.912(8) | 339.391(7) | 339.505(2) | 339.407(2) |
| Rwp (%) | 5.44 | 6.26 | 6.72 | 6.12 | 7.62 | 7.46 | 10.64 |
| χ2 | 5.63 | 4.64 | 4.91 | 4.19 | 5.17 | 4.88 | 7.36 |