**Supplementary Material for “Powder diffraction data on Ca0.9Nd0.1Ti0.9Al0.1O3”**

|  |  |
| --- | --- |
| **Using WinXPOW** | **Using GSAS** |
| Crystal system: Orthorhombic  Space group: Pbnm  *a* = 5.3863(13) Ao  *b* = 5.4344(6) Ao  *c* = 7.6422(11) Ao  Cell Vol. (Å3) = 223.70(5)  Z = 4  Figure of Merit, F(24) = 23.8  DWd = 1.25 | Crystal system: Orthorhombic  Space group: Pbnm  *a* = 5.3832(1) Ao  *b* = 5.4343(1) Ao  *c* = 7.6389(2) Ao  Cell Vol. (Å3) = 223.4677  Z = 4  Calculated unit cell formula weight = 577.205 gm mol-1  ρx = 4.289 g/cm3  *χ*2 = 1.877  R(F2) = 5.60  Rp = 7.92  Rwp = 10.77  DWd = 1.237 |

Table 1: Refined parameters of CNTAO

Table 2: Fractional coordinates used for Rietveld refinement

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Atom | Wyckoff site | X | Y | Z | Occupancy |
| Ca/Nd | 4c | -0.008458 | 0.031675 | 0.25 | 0.9/0.1 |
| Ti/Al | 4b | 0 | 0.5 | 0 | 0.9/0.1 |
| O1 | 4c | 0.061297 | 0.485851 | 0.25 | 1.0 |
| O2 | 8d | 0.712747 | 0.289738 | 0.035099 | 1.0 |

Table 3: Powder diffraction data of CNTAO

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| S.No. | 2θexpt. | Intensity | 2θcal. | Δ2θ | dexpt. | dcal. | (hkl) |
| 1. | 23.220 | 4.8 | 23.232 | -0.0124 | 3.8276 | 3.8256 | (110) |
| 2. | 26.012 | 4.3 | 26.026 | -0.0144 | 3.4228 | 3.4209 | (111) |
| 3. | 33.113 | 100.0 | 33.109 | 0.0038 | 2.7032 | 2.7035 | (112) |
| 4. | 35.007 | 1.8 | 35.020 | -0.0135 | 2.5611 | 2.5602 | (021) |
| 5. | 37.207 | 2.0 | 37.231 | -0.0241 | 2.4146 | 2.4131 | (210) |
| 6. | 39.101 | 6.5 | 39.084 | 0.0172 | 2.3019 | 2.3028 | (103) |
| 7. | 40.714 | 7.4 | 40.713 | 0.0010 | 2.2144 | 2.2144 | (022) |
| 8. | 42.620 | 2.5 | 42.605 | 0.0146 | 2.1196 | 2.1203 | (113) |
| 9. | 44.184 | 1.9 | 44.186 | -0.0018 | 2.0482 | 2.0481 | (122) |
| 10. | 44.335 | 1.9 | 44.363 | -0.0280 | 2.0415 | 2.0403 | (212) |
| 11. | 47.523 | 58.3 | 47.495 | 0.0278 | 1.9117 | 1.9128 | (220) |
| 12. | 49.043 | 3.1 | 49.055 | -0.0125 | 1.8560 | 1.8556 | (221) |
| 13. | 52.158 | 1.1 | 52.170 | -0.0113 | 1.7522 | 1.7519 | (213) |
| 14. | 53.310 | 1.0 | 53.313 | -0.0023 | 1.7170 | 1.7170 | (130) |
| 15. | 54.755 | 3.1 | 54.751 | 0.0035 | 1.6751 | 1.6752 | (131) |
| 16. | 59.045 | 16.2 | 59.059 | -0.0137 | 1.5632 | 1.5629 | (024) |
| 17. | 59.294 | 24.9 | 59.251 | 0.0430 | 1.5572 | 1.5583 | (204) |
| 18. | 65.502 | 1.4 | 65.508 | -0.0054 | 1.4239 | 1.4238 | (133) |
| 19. | 69.067 | 3.0 | 69.080 | -0.0124 | 1.3588 | 1.3586 | (040) |
| 20. | 69.497 | 13.6 | 69.480 | 0.0175 | 1.3515 | 1.3518 | (224) |
| 21. | 73.294 | 1.0 | 73.246 | 0.0480 | 1.2905 | 1.2913 | (323) |
| 22. | 75.552 | 0.8 | 75.529 | 0.0232 | 1.2575 | 1.2578 | (331) |
| 23. | 78.856 | 2.4 | 78.846 | 0.0103 | 1.2129 | 1.2130 | (240) |
| 24. | 79.201 | 7.4 | 79.198 | 0.0034 | 1.2084 | 1.2085 | (116) |