Synthesis and Ab Initio Determination Bi$_{1.256}$ La$_{0.53}$ N$_{0.231}$ O$_{0.521}$ Zr$_{1.543}$ Triclinic Structure from Powder X-Ray Diffraction Data

Bimal K. Kanth, Parashuram Mishra*

Bioinorganic, Materials Chemistry Research Lab. Tribhuvan University, M.M.A.M. Campus, Biratnagar, Nepal

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*Corresponding author: Parashuram Mishra

Abstract

This paper is examined the synthesis and ab initio structure determination of the heavy metal framework mixed valence Bi$_{1.256}$ La$_{0.53}$ N$_{0.231}$ O$_{0.521}$ Zr$_{1.543}$ from precession electron diffraction intensities. The metal framework of the compound was solved in this investigation via direct methods from Powder XRD. A subsequent (kinematical) least-squares refinement with electron intensities yielded slightly improved co-ordinates for the 6 heavy atoms in the structure. Chemical analysis of several crystallites by EDX is in agreement with the formula Bi$_{1.256}$ La$_{0.53}$ N$_{0.231}$ O$_{0.521}$ Zr$_{1.543}$. Moreover, the structure was independently determined by Rietveld refinement from X-ray powder data obtained from a multi-phasic sample. The compound having triclinic crystal system space group P-1 and Centrosymmetry structure with refined lattice parameters a=5.8655, b=4.4099, c=17.6031, α =82.0712, β =88.251 and γ =74.4651. Comparison of the framework structure from electron diffraction with the result from Rietveld refinement shows an average agreement for the heavy atoms within 0.09Å. The titled compound was prepared from mixture of Bi$_2$O$_3$, Zr(NO$_3$)$_4$, and La$_2$O$_3$ by solid state reaction with full thermal decomposition at 1000°C. Rwp = 0.0680, Rp = 0.030 and GOF=0.31 and the structure factors F0 = 2023 and Fc = 2021.

Keywords: Centrosymmetry, X-ray diffraction, EDX, multi-phase, refinement.

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INTRODUCTION

A recent investigation of structural and conductivity properties of Bi$_{1.256}$ La$_{0.53}$ N$_{0.231}$ O$_{0.521}$ Zr$_{1.543}$oxide and nitride conductors (Bi, La and Zr) which belong to the dimorphic tri clinic structural-type family, has proved a close conductivity composition dependence [1]. This has been interpreted on the basis of structural data obtained from Rietveld structure investigations [2]. The structure is built from cationic slabs parallel to (001) faces of the triclinic cells. N and two oxygen sites are located inside; complementary oxide ions, implied by the formulation stoichiometries, are distributed over one or two sites of the inters lab space and exhibit a high mobility, mainly responsible for the conductivity [3]. Depending on the rare-earth nature, at high-temperature form is observed, with a closely hexagonal related structure; its formation from the b2 low-temperature variety occurs during a phase transition that has been attributed to a cationic disordering in the mixed Bi$_3$~/3~3 layers [3]. It is accompanied by sudden increases of both lattice parameters, of oxide occupancy in inter slab spaces, and of the conductivity. The pure iron oxide conductor character of the variety has been clearly demonstrated for the alkaline-earth-based solid solutions and has been also verified for lanthanides-based solid solutions (unpublished results). The thickness of the cationic slabs, which is the largest for the lanthanum term Bi$_{1.256}$ La$_{0.53}$ N$_{0.231}$ O$_{0.521}$ Zr$_{1.543}$ (the best oxide conductor ever evidences in this family), appears to be an important factor for these attractive conductivity properties. Bi$_{1.256}$ La$_{0.53}$ N$_{0.231}$ O$_{0.521}$ Zr$_{1.543}$ a term of a wide Bi1-xLaO1.5 solid solution domain, with 0.154>x0.333, which exhibits anomalies in the evolution of the cell parameters versus composition [5] for one of the particular compositions & Bi$_{1.256}$ La$_{0.53}$ N$_{0.231}$ O$_{0.521}$ Zr$_{1.543}$, a thermal investigation of the quenched to high-temperature form led to evidence of a triclinic crystal system. This paper deals with the ab initio structure determination of this new phase from powder X-ray diffraction data; identification and investigation of the corresponding solid solution, using various techniques such as X-ray diffraction method.
MATERIAL AND METHOD

All chemicals used were analytical grade. A polycrystalline sample of $\text{Bi}_2\text{Zr}_1\text{La}_{0.53}\text{N}_{0.231}\text{O}_{0.521}\text{Zr}_{1.543}$ was synthesized by a standard solid state reaction using a mixture of high purity reagents of $\text{Bi}_2\text{O}_3$, $\text{Zr(NO}_3)_4$ and $\text{La}_2\text{O}_3$ which contained mixed valence as the starting materials in the molar ratio of 1:1:1. The mixture was ground carefully, homogenized thoroughly with methanol (99%) in an agate mortar pestle and then packed into an alumina crucible and calcined at 1000°C in air for 30h with several intermediate grindings [6]. Finally, the product was pressed into pellets and sintered at 100 K/h. Powder X-ray diffraction (XRD) data were collected at room temperature in the angular range of 2θ =10 to 90 with scan step width of 0.02° and a fixed containing time of 15 s using Philips powder diffractometer with graphite monochromatic CuKα radiation. The powder was rotated during the data collection to minimize preferred Orientation effect if any. The program TREOR in CRYSFIRE was used to index the powder pattern which give triclinic cell system. SIRPOW92 was used to locate the positional parameters of constituent atoms. The full pattern is fitting and peak decomposition in the space group $P$-1 using check cell program. The structural parameters were refined by the Rietveld method using the JANA program which gave at 1000°C. $R_{wp} = 0.0680$, $R_p = 0.030$ and $GOF=0.31$ and the structure factors $F_0 = 2023$ and $F_c = 2021$. The density is determined by Archimedes principle.

RESULTS AND DISCUSSIONS

The crystal structure of $\text{Bi}_2\text{Zr}_1\text{La}_{0.53}\text{N}_{0.231}\text{O}_{0.521}\text{Zr}_{1.543}$ is as shown in figure 7. The zirconium occupies the MO6 position in the perovskite layer. However, the continuous O–La–O chains expected in a simple perovskite is disrupted at every $n = 4$ along the $c$ axis by $[\text{Bi}_2\text{O}_2]^{2+}$ layers. The Zr–N distances range from 1×301(4) to 2×557Å with alternate bonds being long and short to result in a zigzag arrangement of $\text{ZrO}_3\text{O}_7$ octahedra [7]. The range of the Zr- N and La–O distances calculated appear to be rather large than those reported in the literature for similar systems. However, more accurate bond lengths have been obtained via neutron diffraction studies for $\text{Bi}_2\text{Zr}_1\text{La}_{0.53}\text{N}_{0.231}\text{O}_{0.521}\text{Zr}_{1.543}$ [8]. The differences in ionic radii of Bi, La and Zr ions also appear to influence the tilt and distortion of the $\text{ZrO}_3\text{O}_7$ octahedra. The Bi–O distances range from 2×25 Å to 3×31 Å. The structure $\text{Bi}_2\text{Zr}_1\text{La}_{0.53}\text{N}_{0.231}\text{O}_{0.521}\text{Zr}_{1.543}$ has three Bi atoms in the asymmetric unit with one of the atoms [Bi(3)] forming the [Bi2O2]2+ layer, while the other two [Bi(1) and Bi(2)] belong to the perovskite layers. Bi (1) and Bi (2) are coordinated to 12 oxygen atoms and Bi(3) is coordinated to 8 oxygens. The structure of $\text{Bi}_2\text{Zr}_1\text{La}_{0.53}\text{N}_{0.231}\text{O}_{0.521}\text{Zr}_{1.543}$ refined using the Rietveld method in the space group $P$-$I$. However, it is noteworthy that earlier reports [10] on thin films of this material demonstrate that it is ferroelectric when grown in specified directions. This suggests the possibility of centrosymmetric arrangements in specific domains in certain crystallographic directions. The occupancy refinements suggest that only in case of $\text{Bi}_2\text{Zr}_1\text{La}_{0.53}\text{N}_{0.231}\text{O}_{0.521}\text{Zr}_{1.543}$ the Zr cations get localized in the Bi2O2 layers. However, it is hard to ascertain this feature since the scattering factors for X-rays for Bi and Zr are nearly the same. On the other hand, it is clear that in the other two compounds the Bi/Zr cations are distributed in both the ZrO3 octahedra. The range of the Zr- N and La–O distances calculated appear to be rather large than those reported in the literature for similar systems. However, more accurate bond lengths have been obtained via neutron diffraction studies for $\text{Bi}_2\text{Zr}_1\text{La}_{0.53}\text{N}_{0.231}\text{O}_{0.521}\text{Zr}_{1.543}$ [8]. The differences in ionic radii of Bi, La and Zr ions also appear to influence the tilt and distortion of the $\text{ZrO}_3\text{O}_7$ octahedra. The Bi–O distances range from 2×25 Å to 3×31 Å. The structure $\text{Bi}_2\text{Zr}_1\text{La}_{0.53}\text{N}_{0.231}\text{O}_{0.521}\text{Zr}_{1.543}$ has three Bi atoms in the asymmetric unit with one of the atoms [Bi(3)] forming the [Bi2O2]2+ layer, while the other two [Bi(1) and Bi(2)] belong to the perovskite layers. Bi (1) and Bi (2) are coordinated to 12 oxygen atoms and Bi(3) is coordinated to 8 oxygens. The structure of $\text{Bi}_2\text{Zr}_1\text{La}_{0.53}\text{N}_{0.231}\text{O}_{0.521}\text{Zr}_{1.543}$ refined using the Rietveld method in the space group $P$-$I$. However, it is noteworthy that earlier reports [10] on thin films of this material demonstrate that it is ferroelectric when grown in specified directions. This suggests the possibility of centrosymmetric arrangements in specific domains in certain crystallographic directions. The occupancy refinements suggest that only in case of $\text{Bi}_2\text{Zr}_1\text{La}_{0.53}\text{N}_{0.231}\text{O}_{0.521}\text{Zr}_{1.543}$ the Zr cations get localized in the Bi2O2 layers. However, it is hard to ascertain this feature since the scattering factors for X-rays for Bi and Zr are nearly the same. On the other hand, it is clear that in the other two compounds the Bi/Zr cations are distributed in both the Bi2O2 and the perovskite layers. Table 2 provides a list of valence bond sums [11] in all these three structures, which indicate a measure of the extent of disorder in these phases. It also compares the tendency of the three oxides to incorporate A type cations in the [Bi2O2] layer and the perovskite layers [12].

Fig-1: Powder XRD spectra of $\text{Bi}_2\text{Zr}_1\text{La}_{0.53}\text{N}_{0.231}\text{O}_{0.521}\text{Zr}_{1.543}$
Crystal structures

High-resolution data set was collected for Bi$_{1.256}$La$_{0.53}$N$_{0.231}$O$_{0.521}$Zr$_{1.543}$ on a Philips powder diffractometer utilizing CuKα radiation. The refinement was done using the JANA2006 software. As in the case of Bi$_{1.256}$La$_{0.53}$N$_{0.231}$O$_{0.521}$Zr$_{1.543}$, indexing the powder patterns was not straightforward as two sets of Miller indices are possible for the strongest reflections yielding two alternative unit cells which led to close residuals upon LeBail full-pattern decomposition. Subsequent Rietveld refinements clearly ruled out one of these due to intolerably dissimilar La–O distances in the Bi$_2$O$_3$ anion. Final Rietveld refinement plot for Bi$_{1.256}$La$_{0.53}$N$_{0.231}$O$_{0.521}$Zr$_{1.543}$ is given in Figure 3; general projection of the Perovskite crystal structure is shown in Figure 2; the refinement results are collected in Tables 1. For Bi$_{1.256}$La$_{0.53}$N$_{0.231}$O$_{0.521}$Zr$_{1.543}$ structures was refined from routine XRD data to confirm the same atomic arrangement; these refinements also converged to reasonable R values. Just traces of by-products were present which could not be identified as their estimated content is below 1%.

Fig-2: Rietveld refinement of Bi$_{1.256}$La$_{0.53}$N$_{0.231}$O$_{0.521}$Zr$_{1.543}$

Fig-3: Perovskite structure of Bi$_{1.256}$La$_{0.53}$N$_{0.231}$O$_{0.521}$Zr$_{1.543}$
Fig. 3: General projection of polyhedron type structure of Bi$_{1.256}$La$_{0.53}$N$_{0.231}$O$_{0.521}$Zr$_{1.543}$

Table 1: Crystallographic data after Rietveld refinement

| Formula sum       | Bi$_{1.256}$La$_{0.53}$N$_{0.231}$O$_{0.521}$Zr$_{1.543}$ |
|--------------------|----------------------------------------------------------|
| Formula weight     | 488.4 g/mol                                               |
| Crystal system     | Triclinic                                                 |
| Space group        | P - 1 (2)                                                 |
| Cell parameters    | a=5.0302 Å, b=7.2625 Å, c=8.3400 Å, α=74.3014°, β=84.4133°, γ=74.2675° |
| Cell ratio         | a/b=0.6926, b/c=0.8708, c/a=1.6580                       |
| Cell volume        | 282.23 Å$^3$                                             |
| Z                  | 2                                                        |
| Calc. density      | 5.74684 g/cm$^3$                                         |
| Meas. density      | 5.7659 g/cm$^3$                                          |
| Pearson code       | aP43                                                     |
| Formula type indexes | N2O4P6Q6R25               |
| Wyckoff sequence   | i21f                                                     |

Table 2: Fraction Atomic parameters

| Atom | Ox. | Wyck. | Site | S.O.F. | x/a | y/b | z/c | U [Å$^2$] |
|------|-----|-------|------|--------|-----|-----|-----|-----------|
| Bi1  | 3   | 2i    | 1    | -0.00536 | 0.10643 | 0.20272 | 0.0380 |
| La1  | 3   | 2i    | 1    | -0.66940 | 0.30889 | 0.87557 | 0.0380 |
| La2  | 3   | 2i    | 1    | -1.02512 | 0.57776 | 0.25255 | 0.0380 |
| La3  | 3   | 2i    | 1    | -0.41060 | 0.19881 | 0.42437 | 0.0380 |
| Zr1  | 4   | 2i    | 1    | -0.57773 | 0.24545 | 0.53666 | 0.0380 |
| Zr2  | 4   | 2i    | 1    | -0.71116 | 0.60189 | 0.18303 | 0.0380 |
| Zr3  | 4   | 2i    | 1    | -0.76396 | 0.43947 | 0.24622 | 0.0380 |
| Zr4  | 4   | 2i    | 1    | -0.52333 | 0.34626 | 0.04873 | 0.0380 |
| Zr5  | 4   | 2i    | 1    | -0.53518 | 0.20067 | 0.76182 | 0.0380 |
| Zr6  | 4   | 2i    | 1    | -0.67793 | 0.40350 | 0.33281 | 0.0380 |
| Zr7  | 4   | 2i    | 1    | -0.29135 | 0.17799 | 0.10042 | 0.0380 |
| Zr8  | 4   | 2i    | 1    | -0.87047 | 0.29054 | 0.28411 | 0.0380 |
| Zr9  | 4   | 2i    | 1    | -0.53782 | 0.10083 | 0.96235 | 0.0380 |
| Zr10 | 4   | 1f    | -1   | -1/2    | 0      | 1/2   | 0.0380 |
| Zr11 | 4   | 2i    | 1    | 0.30565 | -0.01498 | 0.15334 | 0.0380 |
| Zr12 | 4   | 2i    | 1    | -0.31980 | 0.42431 | 0.49792 | 0.0380 |
| Zr13 | 4   | 2i    | 1    | 0.23623 | 0.01199 | 0.35639 | 0.0380 |
| O1   | 2   | 2i    | 1    | -0.16966 | 0.22472 | 0.33583 | 0.0380 |
| O2   | 2   | 2i    | 1    | -0.11962 | -0.09476 | 0.13916 | 0.0380 |
| N1   | 3   | 2i    | 1    | -0.88339 | 0.41703 | 0.08263 | 0.0380 |
| N2   | 3   | 2i    | 1    | -0.12394 | -0.14891 | 0.32576 | 0.0380 |
| N3   | 3   | 2i    | 1    | -0.10011 | 0.37329 | 0.09634 | 0.0380 |
## Table-3: Selected bond angles

| Atom 1 | Atom 2 | Atom Code 1 | Atom Code 2 | Bond angle |
|--------|--------|-------------|-------------|------------|
| Bi1    | O1     | 18555011    | Zr7         | 87.657     |
| Bi1    | O1     | 18555011    | Zr11        | 142.246    |
| Bi1    | O1     | 18555011    | Zr13        | 82.017     |
| Bi1    | O1     | 18555011    | N3          | 71.966     |
| Bi1    | O1     | 18555011    | O2          | 124.559    |
| Bi1    | O1     | 18555011    | Zr8         | 55.503     |
| Bi1    | O1     | 18555011    | N2          | 92.567     |
| Bi1    | O1     | 18555011    | N1          | 81.950     |
| La1    | Zr7    | 11555011    | Zr11        | 129.753    |
| La1    | Zr7    | 11555011    | Zr13        | 164.067    |
| La1    | N3     | 22555011    | O2          | 125.363    |
| La1    | N3     | 22555011    | Zr8         | 60.076     |
| N3     | N3     | 22555011    | N2          | 149.571    |
| N3     | N3     | 22555011    | N1          | 28.894     |
| N3     | O1     | 19456021    | Zr2         | 44.622     |
| La2    | Zr5    | 9555011     | La2         | 92.393     |
| La2    | Zr5    | 9555011     | O2          | 68.926     |
| La2    | Zr9    | 13555011    | La2         | 132.607    |
| La2    | Zr9    | 13555011    | O2          | 64.325     |
| La2    | Zr9    | 13555011    | Zr2         | 95.447     |
| La2    | Zr9    | 13550011    | N1          | 100.488    |
| La2    | Zr9    | 13550011    | N3          | 146.472    |
| La2    | La2    | 3366021     | N3          | 66.902     |
| La2    | La2    | 3366021     | Zr11        | 125.495    |
| O2     | Zr3    | 19456021    | Zr2         | 44.622     |
| N3     | Zr9    | 22466021    | Zr11        | 162.579    |
| La3    | Zr3    | 7555011     | Zr2         | 46.610     |
| La3    | Zr3    | 7555011     | La1         | 137.766    |
| La3    | Zr3    | 7555011     | N1          | 51.896     |
| La3    | Zr3    | 7555011     | N2          | 129.414    |
| La3    | Zr3    | 7555011     | O2          | 126.029    |
| La3    | Zr3    | 7555011     | N3          | 75.341     |
| La3    | Zr6    | 2366021     | Zr5         | 36.613     |
| La3    | Zr6    | 10555011    | Zr8         | 47.297     |
| N1     | N1     | 20555011    | Zr5         | 124.474    |
| N2     | N2     | 21465011    | O2          | 39.792     |
| N2     | N2     | 21465011    | N3          | 52.401     |
| N2     | N2     | 21465011    | Zr5         | 55.077     |
| O2     | O2     | 19465011    | Zr5         | 118.897    |
| O2     | O2     | 19465011    | Zr2         | 54.244     |
| N3     | N3     | 22455011    | Zr5         | 99.525     |
| La3    | Zr1    | 5555011     | O1          | 145.411    |
| La3    | Zr1    | 5555011     | Zr10        | 79.278     |
| Zr6    | Zr6    | 10555011    | Zr12        | 78.383     |
| Zr6    | Zr6    | 10555011    | Zr13        | 148.425    |
| Zr1    | La1    | 4555011     | Zr6         | 67.615     |
| Zr1    | La1    | 4555011     | Zr10        | 58.322     |
| Zr1    | La1    | 4555011     | Zr10        | 58.322     |
| N2     | N2     | 21465021    | Zr13        | 96.571     |
| N2     | N2     | 21465021    | Zr12        | 107.508    |
| Zr12   | Zr12   | 16555011    | Zr13        | 90.866     |
| Zr12   | Zr12   | 16555011    | Zr12        | 59.934     |
| Zr12   | Zr12   | 17566021    | Zr12        | 136.453    |
| Zr2    | Zr3    | 7555011     | Zr6         | 30.028     |
| Zr3    | Zr3    | 7550011     | La2         | 56.513     |
| Zr3    | Zr3    | 7550011     | Zr6         | 126.308    |
| O1     | O1     | 4555011     | Bi1         | 155.591    |
| O1     | O1     | 4555011     | Zr8         | 159.757    |
| O1     | O1     | 4555011     | N3          | 131.075    |
| O1     | O1     | 4555011     | Zr12        | 66.452     |
| O1     | O1     | 4555011     | Zr13        | 127.375    |
| O1     | O1     | 4555011     | Zr7         | 95.178     |
| Bi1    | Bi1    | 1555011     | Zr8         | 59.564     |
| Bi1    | Bi1    | 1555011     | N3          | 166.607    |
| N1     | N3     | 22455011    | Zr3         | 117.790    |
| N1     | N3     | 22455011    | Zr8         | 80.646     |
| N1     | N3     | 22455011    | Zr4         | 147.681    |
| N1     | N3     | 22455011    | N3          | 108.028    |
| N1     | N3     | 22455011    | N1          | 69.545     |
| N1     | N3     | 22455011    | La2         | 89.041     |
| N1     | N3     | 22455011    | Zr2         | 135.809    |
| N1     | N3     | 22455011    | La1         | 104.767    |
| N1     | N3     | 22455011    | Zr6         | 117.167    |
| N1     | N3     | 22455011    | Bi1         | 48.004     |
CONCLUSIONS

In summary, it may be stated that the room temperature crystal structures of three \( n = 4 \) Perovskite types of oxides have been refined from high resolution X-ray diffraction data. The pattern decomposition and peak extraction methods have been used for the first time to derive starting models for \( \text{Bi}_2\text{La}_{0.5}\text{Ni}_{0.5}\text{O}_{3} \) and \( \text{Zr}_3\text{Ti}_5\text{O}_{15} \). A model has been proposed for this high temperature phase. It is also confirmed that the ferroelectric to paraelectric phase transition in \( \text{Bi}_2\text{La}_{0.5}\text{Ni}_{0.5}\text{O}_{3} \) is accompanied by a structural phase transition. The zigzag arrangement of the distorted \( [\text{ZrO}_4] \) octahedral and \( \text{LaNi} \) is tetrahedral as observed in the \( n = 2 \) series of Perovskite phases are found in these structures as well. A rational explanation for the distribution of the \( \text{Bi}^3\text{Zr}^4\text{La}^4 \) cations in the A sites as well as the \( [\text{Bi}_2\text{O}_2] \) sites is provided based on the VBS calculations. \( \text{Bi}_2\text{La}_{0.5}\text{Ni}_{0.5}\text{O}_{3} \) shows a structural transition to the prototype triclinic structure in the space group \( P-1 \). A model has been proposed for this high temperature phase. It is also confirmed that the ferroelectric to paraelectric phase transition in \( \text{Bi}_2\text{La}_{0.5}\text{Ni}_{0.5}\text{O}_{3} \) by a structural phase transition.

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