


 Cite this: *RSC Adv.*, 2025, 15, 5232

## Reply to the 'Comment on "Investigation of the structural, surface topographical, fractal, capacitive, and electrical properties of a defect brownmillerite perovskite material $\text{KBiFeMnO}_5$ for electronic devices" by P. Tomaszewski, *RSC Adv.*, 2024, DOI: 10.1039/D4RA04218B'

 Debasish Panda,  Sudhansu Sekhar Hota \* and Ram Naresh Prasad Choudhary

This reply mainly deals with the scientific description of the comments on the structure of the published compound  $\text{KBiFeMnO}_5$ . The newly developed compound was prepared using a standard ceramic technology (high-temperature solid-state reaction technique). The high-purity ingredients ( $\text{K}_2\text{CO}_3$ ,  $\text{Bi}_2\text{O}_3$ ,  $\text{Fe}_2\text{O}_3$  and  $\text{Mn}_2\text{O}_3$ ) were taken stoichiometrically to create a single-phase compound, whereas, in the commented article,  $\text{KBiFeMnO}_5$  is written as sillenite  $\text{Bi}_{25}\text{FeO}_{40}$  or/and  $\text{Bi}_{24}\text{Mn}_2\text{O}_{40}$  that is unacceptable without other detailed experiments.

Received 6th August 2024

Accepted 6th February 2025

DOI: 10.1039/d4ra05696e

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The present article mainly deals with the scientific incorrectness raised by Paweł E. Tomaszewski in the published article.<sup>1</sup> The defect type of brownmillerite ceramic  $\text{KBiFeMnO}_5$  (KBFMO) was prepared *via* solid-state reaction technique taking the stoichiometric ingredients ( $\text{K}_2\text{CO}_3$ ,  $\text{Bi}_2\text{O}_3$ ,  $\text{Fe}_2\text{O}_3$  and  $\text{Mn}_2\text{O}_3$ ). In the published paper, the structural properties were scientifically analysed. It is written that the material KBFMO has a distorted structure, which is compatible with all the properties. Unfortunately, the author addressed that the X-ray diffraction (XRD) pattern is sillenite phase ( $\text{Bi}_{25}\text{FeO}_{40}$  or/and  $\text{Bi}_{24}\text{Mn}_2\text{O}_{40}$ ). It should be noted that the sillenite should be prepared with different amounts of stoichiometric ingredients that could not be the same as the KBFMO ceramic. Comparing an XRD pattern needs similar Bragg's angles, intensities, and width of the peaks, but interestingly, in Fig. 1, comparing pictures for a scientific article without proper scientific experiments is not acceptable.

It should be noted that a proper phase analysis needs all accurate XRD peaks, but unfortunately, the author reported that many peaks of the parent phase KBFMO are matched with some sillenite phase. That does not mean that the sillenite and KBFMO compounds are the same. Splits of the peaks and width are the cause of the structural changes.<sup>2</sup>

It should be noted that for a single-phase analysis, all peaks should be mentioned. Without all peaks analysis, the reporting phase is not acceptable. The reported XRD pattern is analysed using the Monte Carlo, PIRUM, and Le Bail techniques in EXPO

software.<sup>3</sup> It is a powerful tool at the end of the elaborate crystal structure solution. Without sufficient knowledge, the analysis of the structure is very difficult.

To evaluate the crystal system there is various methods and tools are used such as;

- (1) Lzon612 (Robin Shirley & Daniel Louër)<sup>4</sup>
- (2) Dicvol91 (D. Louër)<sup>5</sup>
- (3) Ito12 (Jan Visser)<sup>6</sup>
- (4) Treor90 (Per-Eric Werner)<sup>7</sup>
- (5) Taup (Daniel Taupin)<sup>8</sup>
- (6) FJZN (Jan Visser & R. Shirley)
- (7) Kohl (Franz Kohlbeck)<sup>9</sup>
- (8) LOSHFZRF (Daniel Louër & Robin Shirley)<sup>10</sup>
- (9) McMaille (Monte Carlo powder indexing program by Armel Le Bail)<sup>11</sup>

All these method and tools are used for the identification of the new crystal system. The use of TREOR and McMaille methods are consistent for the investigation of the crystal system by analysing Bragg's angle with intensity.<sup>12</sup> Rietveld (with CIF data) and Le Bail (no CIF data) refinement have also consistent for structural analysis.<sup>13</sup>

Another interesting comment of the author is correlating structure of all the similar groups of the brownmillerite compounds. It is noted that the brownmillerite phase correlates with the KBFMO structure in the published article, which may be overlooked. Different substituting elements in different sites on an atom have different structures. However, similar compounds for doping elements are mandatory for comparing the structural stability, but in the present published article,

Physics Department, Siksha 'O' Anusandhan (deemed to be) University, Bhubaneswar 751030, India. E-mail: [sudhansusekhar405@gmail.com](mailto:sudhansusekhar405@gmail.com)



unique structural and functional properties have not been reported before.

In the published article, surface topology and microstructural properties were extensively analysed. It is noted that the material is polycrystalline in nature, which corresponds to different grains and grain boundaries. After the colour mapping of all constituent elements K, Bi, Fe, Mn, and O, the presence of all elements is verified. Interestingly, by not taking atom probe tomography, it could not identify non-presence Bi atom and parasite phase from the SEM image of the published paper Fig. 2(a).

Most important rules of the crystallography are;

1. Extra peaks and secondary phases can affect the crystal structure of a material.
2. Impurities can occupy lattice sites substituting for native atoms form interstitial defects and distorting the lattice, such as lattice constant, cell volume. It can alter the bonding between atoms, changing the crystal structure.
3. Secondary phases can have a different crystal structure than the primary phase form interfaces with the primary phase, disrupting the crystal structure.
4. Other phases can segregate at grain boundaries affecting the crystal structure and properties.
5. Impurities and secondary phases can introduce defects, such as vacancies, dislocations, and stacking faults, which can alter the crystal structure.

Here the commented paper is differ from the fundamental rules that's why these analysis have no scientific value.

Lastly, it should be noted that the JCPDS/ICDD file is not available for every compounds. A file/pattern may partially match with sillenite compounds, which is not the same compound of KBFMO. Once again, the author has not done any other experiments to check the correctness of the structure. Thus, the reported structural analysis in the published paper<sup>1</sup> is correct and acceptable, as confirmed by the results of other experimental techniques (dielectric and electrical properties).

## Data availability

The data will be available at a reasonable request.

## Conflicts of interest

The author declares that he has no known competing financial interests or personal relationships that could have appeared to influence the work.

## References

- 1 D. Panda, S. S. Hota and R. N. P. Choudhary, Investigation of the structural, surface topographical, fractal, capacitive, and electrical properties of a defect brownmillerite perovskite material  $\text{KBiFeMnO}_5$  for electronic devices, *RSC Adv.*, 2024, **14**(5), 3400–3412.
- 2 T. Egami and S. J. Billinge, *Underneath the Bragg Peaks: Structural Analysis of Complex Materials*, Elsevier, 2003, vol. 16.
- 3 A. Altomare, F. Capitelli, N. Corriero, C. Cuocci, A. Falcicchio, A. Moliterni and R. Rizzi, The Rietveld refinement in the EXPO software: a powerful tool at the end of the elaborate crystal structure solution pathway, *Crystals*, 2018, **8**(5), 203.
- 4 R. Shirley and D. Louër, New powder indexing programs for any symmetry which combine grid-search with successive dichotomy, *Acta Crystallogr.*, 1978, **34**, 382.
- 5 A. Boulouf and D. Louër, Indexing of powder diffraction patterns for low-symmetry lattices by the successive dichotomy method, *J. Appl. Crystallogr.*, 1991, **24**, 987–993.
- 6 J. W. Visser, A Fully Automatic Program for Finding the Unit Cell from Powder Data, *J. Appl. Crystallogr.*, 1969, **2**, 89–95.
- 7 P.-E. Werner, L. Eriksson and M. W. TREOR, a Semi-Exhaustive Trial-and-Error Powder Indexing Program for All Symmetries, *J. Appl. Crystallogr.*, 1985, **18**, 367–370.
- 8 D. Taupin, A Powder-Diagram Automatic-Indexing Routine, *J. Appl. Crystallogr.*, 1973, **6**, 380–385.
- 9 F. Kohlbeck and E. M. Hörl, Trial and error indexing program for powder patterns of monoclinic substances, *J. Appl. Crystallogr.*, 1978, **11**, 60–61.
- 10 R. Shirley and D. Louër, New powder indexing programs for any symmetry which combine grid-search with successive dichotomy, *Acta Crystallogr.*, 1978, **34**, 382.
- 11 A. Le Bail, Monte carlo indexing with mcmaille, *Powder Diffr.*, 2004, **19**(3), 249–254.
- 12 D. Panda, S. S. Hota and R. N. P. Choudhary, Synthesis of a scheelite barium molybdate: structural, topological, electrical, and transport properties for negative temperature coefficient thermistor application, *J. Solid State Chem.*, 2024, **331**, 124531.
- 13 D. Panda, S. S. Hota and R. N. P. Choudhary, Investigation of structural, topological, and electrical properties of scheelite strontium molybdate for electronic devices, *Inorg. Chem. Commun.*, 2023, **158**, 111501.

