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COMMENT

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Comment on "Investigation of the structural, surface topographical, fractal, capacitive, and electrical properties of a defect brownmillerite perovskite material $KBiFeMnO_5$ for electronic devices" by D. Panda, S. S. Hota and R. N. P. Choudhary, *RSC Adv.*, 2024, 14, 3400

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The comments present the erroneous processing of diffraction data. The 'novel' complex material $KBiFeMnO_5$ described in the commented paper does not exists at all. The studied sample was mainly the sillenite $Bi_{25}FeO_{40}$ or/and $Bi_{24}Mn_2O_{40}$ instead of brownmillerite $KBiFeMnO_5$. Thus, the data from subsequent experiments are without scientific value.

There are many papers by the team of R. N. P. Choudhary devoted to introducing new compounds. Three of them are devoted to different brownmillerite materials, $A_2B_2O_5$, as deemed by authors. The commented paper describes the sample supposed to be of $KBiFeMnO_5$.[1] Unfortunately, the simple analysis of the diffraction pattern shown in Fig. 1a of the commented paper clearly indicates that the sample is a mixture of at least two crystals. The majority part of the sample consists of the sillenite crystal $Bi_{25}FeO_{40}$ or/and $Bi_{24}Mn_2O_{40}$. It should be noted that the diffraction pattern of a mixture of crystalline phases is a sum of their diffraction patterns. Thus, if we find the set of diffraction peaks well matching to given crystal (the same positions and the same intensities), such crystal is present in the sample. This is a case of the sample studied by authors. The other small peaks (for example at about $2\theta \sim 25$, 32, 37°) must correspond to some impurity phase more probably containing K-ions. Unfortunately, the poor quality of the figure prevent the finding of the chemical composition of this supplementary phase (the points market by big circles don't allow to measure of the 2θ angles). Fig. 1 can permit the direct comparison of both patterns, experimental and that of sillenite phase.

It should be noted that the nearly all experimental peaks are highest than those calculated by authors. Such effect may be due to the width of the calculated peaks too high.

It should be noted that the indexation using all diffraction peaks is wrong procedure in the case of mixture of crystals. Thus, the presented values of lattice parameters are not correct. This is supported by high value of reliability factors indication on erroneous analysis. Modern analyses are possible especially for so clear diffraction pattern as in the commented case. It should be also noted, that the data on so high degree of Chebyshev polynomial as well as so many parameter of profile peak shape function give no interesting and valuable information.

The very similar situation one can find in two other paper from the same team of authors.[2,3] The first is not $LiBiFe_2O_5$ and the second $KBiMn_2O_5$. Both contains the sillenite phases: $Bi_{25}FeO_{40}$, and $Bi_{24}Mn_2O_{40}$, respectively, with some admixture of other unknown phases. It should be underline that authors did not made any comparison of these three samples what is a good policy of scientific analysis of samples of so similar supposed composition.

There is also some inconsistences on the chemical composition presented in Fig. 2f of the commented paper. The distribution of all ions is not the same suggesting the different chemical composition. For example, the two big grains seen on Fig. 2a of the commented paper do not have Bi-atoms and can be of parasite phase.

It should be noted that the lack of the compatibility of the chemical composition of the ingredients used and the formula of main crystal phase as shown above, can't be used to postpone the above analysis of the diffraction pattern. It is well known that the crystal growth, a kind of art, requires some non-stoichiometric composition of starting compounds (for example some excess of one component or even other compounds) necessary to obtain the crystal of desired formula. The simple summation of chemical formula as made by authors is not sufficient.

Data availability

The data will be available on reasonable request.

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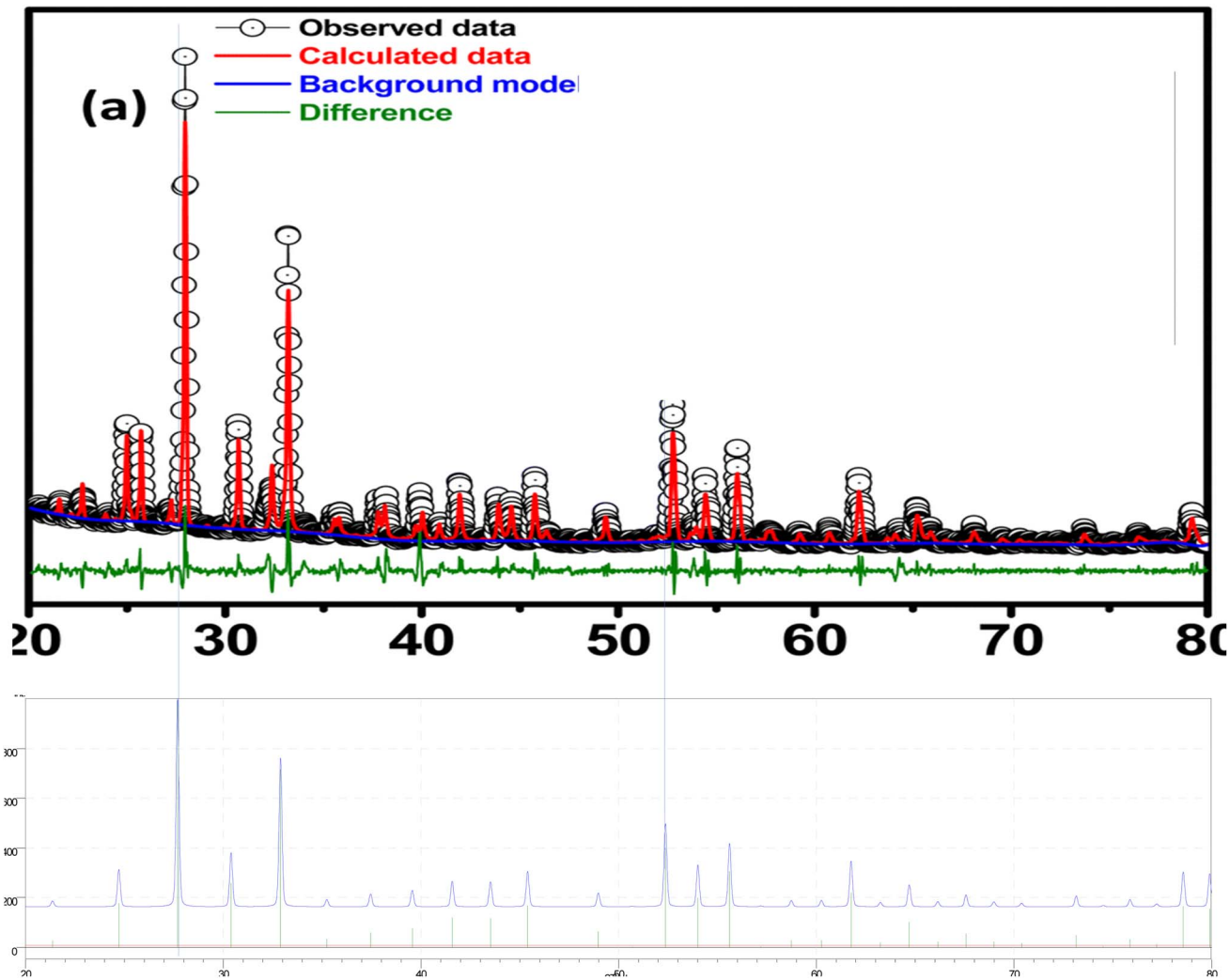

Fig. 1 The comparison of both patterns, experimental (upper diagram) and that of sillenite phase $Bi_{25}FeO_{40}$ or $Bi_{24}Mn_2O_{40}$ (bottom pattern, ICSD #41937 and ICSD #75390, respectively; both have nearly the same diffraction pattern). Note that the 2θ-scale is the same for both patterns.

Author contributions

All the content of the presented paper is my own contribution.

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 $KBiFeMnO_5$ for electronic devices, *RSC Adv.*, 2024, **14**, 3400–3412, DOI: **10.1039/D3RA08106K**.

2 D. Panda, S. S. Hota and R. N. P. Choudhary, A brownmillerite electronic material $LiBiFe_2O_5$: structural, dielectric, electrical, and ferroelectric properties for device application, *Phase Transitions*, 2023, **96**, 822–839, DOI: **10.1080/01411594.2023.2272015**.

3 D. Panda, S. S. Hota and R. N. P. Choudhary, Structural, morphological, dielectric, and electrical characteristics of a brownmillerite material for electronic devices: $KBiMn_2O_5$, *Chem. Phys. Impact*, 2024, **8**, 100540, DOI: **10.1016/j.chphi.2024.100540**.