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Effect of temperature and theoretical-experimental GAP analysis on BiFeO3 nanoparticles

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Summary

Bismuth ferrite $BiFeO_3$ is a multifunctional material called multiferroic, this material has attracted great interest in scientists due to its potential applications in information storage devices, sensors and photovoltaics [1].

In this work, $BiFeO_3$ has been synthesized and characterized by the combustion method in solution, the sample obtained in $BiFeO_3$ powder underwent heat treatment at 500 °C and 600 °C. The samples were structurally characterized by means of a ray diffractometer. The Rietveld refinement was used to adjust the simulated DRX diffraction pattern to the experimental one to obtain with greater precision the lattice parameters and atomic positions. The unit cell of $BiFeO_3$ was visualized from the refined cell parameters by the VESTA software. The calculation of the forbidden band has been carried out using the diffuse reflectance spectrum based on the theory of the Kubelka-Munk function and the Tauc equation. By calculating its total and partial state density, the forbidden band was checked [2].

Method

Figure 1: Heat treatment process

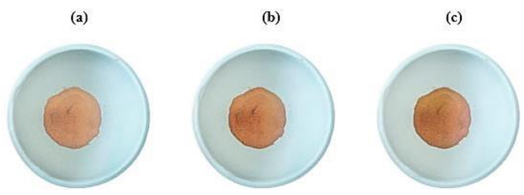


Figure 2: Staining of the $BiFeO_3$ samples: a) $BiFeO_3$ without heat treatment, b) $BiFeO_3$ with heat treatment at 500 °C and c) $BiFeO_3$ with heat treatment at 600 °C.

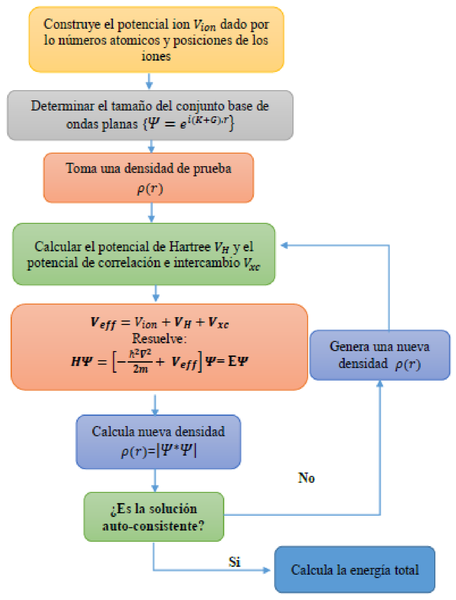
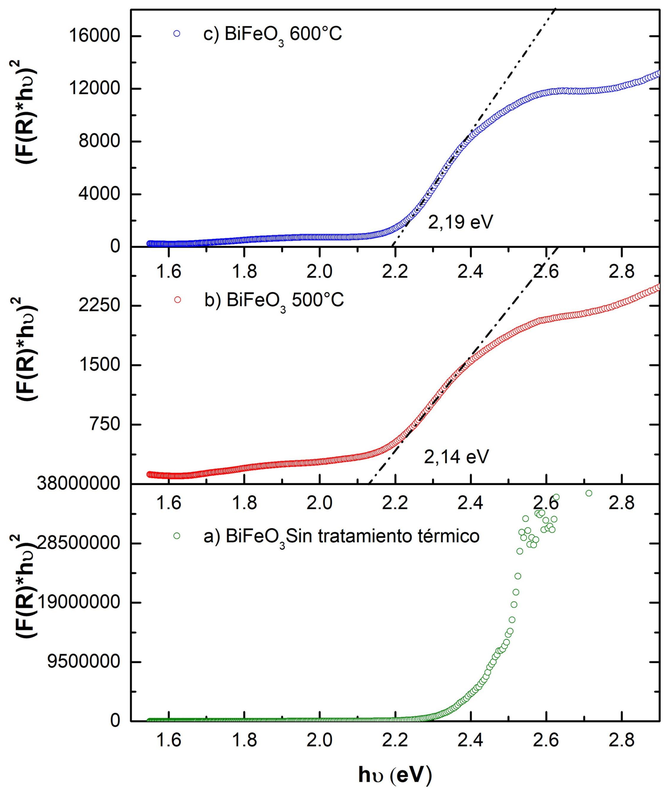


Figure 3: Schematic diagram of the auto cycle consisting of the calculation of total energy in Quantum Espresso

Results

Figure 4: a) Rietveld refinement of $BiFeO_3$ diffractograms, b) Representation of the unit cell by VESTA software and c) Enlarged view of two interconnected neighboring octahedra of FeO_6

In the diagrams presented, the information of the crystalline structure (hexagonal) and single phase of $BiFeO_3$ adjusted with the hexagonal structure of the space group R3c is observed, which exactly matches the values of the literature [3] . Likewise, the angles between the Fe-O-Fe atoms can be visualized, which is related to the energy of the forbidden band of $BiFeO_3$, this angle is seen to grow due to the thermal treatment carried out on the material, which confirms a better obtaining of the GAP. The relationship is defined at a higher heat treatment temperature, the Fe-O-Fe angle increases and therefore the GAP decreases. It can also be seen that the optimum heat treatment temperature was 500° C.



Optical Characterization

The forbidden energy band (GAP) was obtained by taking the part that allows a linear fit in the graphs $(F(R)hv)^2$ vs hv el , which is extrapolated to the abscissa axis. The GAP value among the 3 samples analyzed, it is observed that it decreases when the heat treatment temperature increases, reaching an optimum value of 500 °C, because 600 °C the GAP value stabilizes. The values are comparable with the data reported by other studies [4].

Figure 5: Tauc graph for the calculation of the forbidden energy band, direct electronic transition: a) $BiFeO_3$ without heat treatment, b) $BiFeO_3$ with heat treatment at 500 °C and c) $BiFeO_3$ with heat treatment at 600 °C.

Quantum Espresso Simulation: Density of States

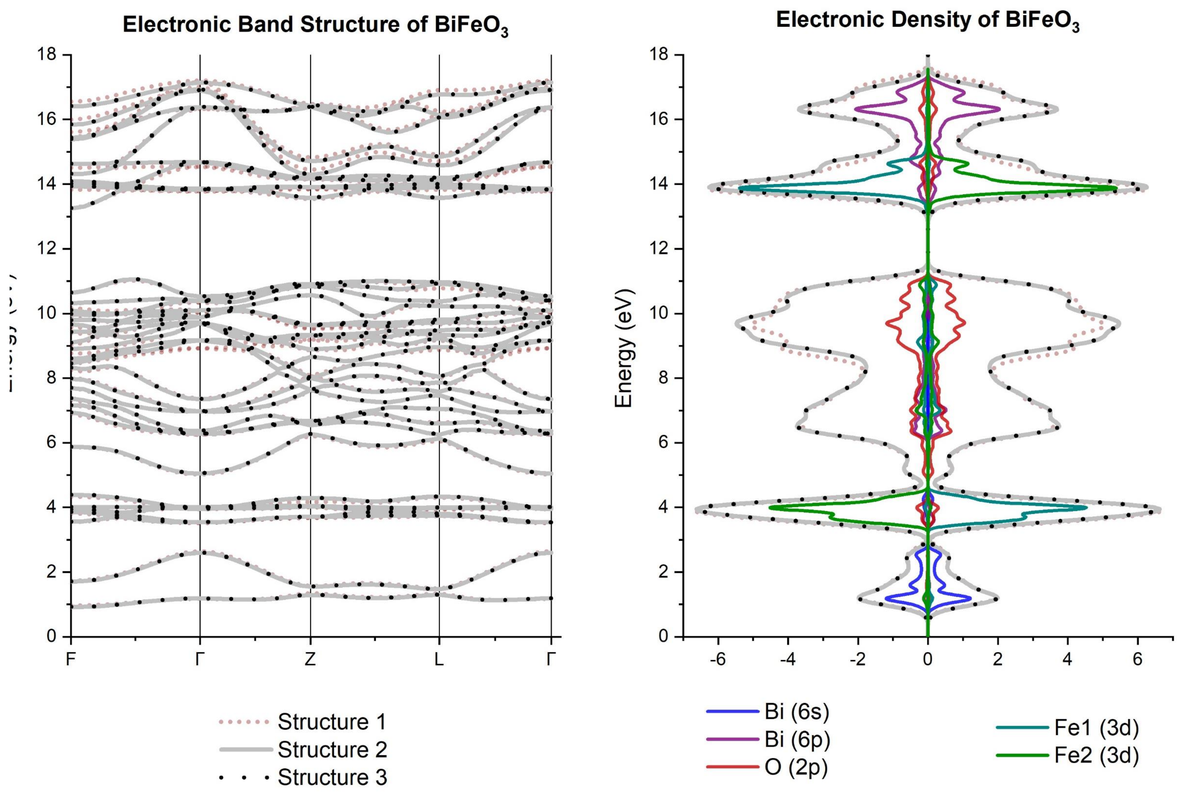


Figure 6: Density of total and partial states of $BiFeO_3$

In the total and partial state density graph, the maximum valence band formed by the O_{2p} state is observed, the minimum conduction band above the fermi energy is constituted by the mixture of the Fe_{3d} states with small contributions from the O_{2p} state . Between the states O_{2p} and Fe_{3d} no state is observed, indicating a prohibited energy of 2,1 eV which is approximate to the experimental value found, of 2.14 eV of the graph figure 4. A greater intensity of the state Bi_{6s} is appreciated around 2 eV, also you can observe a mixture of states between the Fe_{3d} state and the O_{2p} state at 4 eV indicating the hybridization between these states. These values are comparable with the data reported in other investigations [5].

Conclusions

- The diffraction peaks are highly compatible with the presence of the $BiFeO_3$ phase with hexagonal structure and R3c group space. The DRX $BiFeO_3$ pattern is refined by the Full Prof Suit software, the pattern clearly indicates good crystallization of the $BiFeO_3$ phase.
- In the $BiFeO_3$ nanoparticles with a thermal treatment at 500 °C, we found an optimal forbidden band of 2.14 eV, it is an improvement to the values reported by other authors. The synthesis method, heat treatment and purity in the phase influence this value.
- In the computational calculations on Quantum Espresso for the determination of the forbidden band, the parameter U = 5 was used in the Fe atom generating a correction to the dd states of the Fe with which the forbidden bandwidth of $BiFeO_3$ was determined, obtaining a value Eg = 2.1eV between the states O_{2p} and Fe_{3d}, this being close to the value obtained by diffuse reflectance. In addition, it was identified that the maximum valence band formed by the O_{2p} state and the minimum conduction band formed by the Fe_{3d} state and small contributions from the O_{2p} state.

references

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