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Preparation of new perovskite ferroelectric compound

Harith M. Saeed[1*], Emad AlShakarchi[2]
[1,2]Al-Nahrain University, Iraq; harith.m.s.h@gmail.com (H.M.S.) Esk2000@hotmail.com (E.A.S.)

Abstract: The main objective of the research is to prepare a new ferroelectric compound with a perovskite phase. This is done by mixing several materials of different phases and with different concentrations to prepare that new intended compound by solid state reaction method; Using the Phase diagram, each of its three angles represents a compound of one of the three ferroelectric compounds $Batio_3$, $BiNatio_3$ and $BiLitio_3$. Then, through the specified area, called morphotropic phase Boundary three points (arbitrary Points) are taken, the point one was ($Bi_{0.48175}$ $Na_{0.465}$ $Li_{0.001675}$ $Ba_{0.0365}$ Tio_3), point two was ($Bi_{0.48675}$ $Na_{0.475}$ $Li_{0.01175}$ $Ba_{0.0265}$ Tio_3) and point three was ($Bi_{0.492}$ $Na_{0.485}$ $Li_{0.007}$ $Ba_{0.016}$ Tio_3) that are projected onto the Phase Diagram coordinates to find out.
Keywords: *Ferroelectric, MPB, New compound, Perovskite, Solid state reaction method.*

1. Introduction

Ferroelectricity is a property of certain materials that have a spontaneous electric polarization that can be reversed by the application of an external electric field. The term is used in analogy to ferromagnetism, in which a material exhibits a permanent magnetic moment.

Ferromagnetism was already known when ferroelectricity was discovered in 1920 in Rochelle salt by Valasek. Thus, the prefix Ferro, meaning iron, was used to describe the property despite the fact that most ferroelectric (FE) materials do not contain iron [1],[2].

FE materials – for example, barium titanate (BaTiO3) and Rochelle salt – are composed of crystals in which the structural units are tiny electric dipoles; that is, in each unit the centers of positive charge and of negative charge are slightly separated.

In some crystals these electric dipoles spontaneously line up in clusters called domains, and in FE crystals the domains can be oriented predominantly in one direction by a strong external electric field [3],[4].

Reversing the external field reverses, the predominant orientation of the FE domains, though the switching to a new direction lag somewhat behind the change in the external electric field [5].

This lag of electric polarization behind the applied electric field is FE hysteresis, named by analogy with ferromagnetic (FM) hysteresis. Ferroelectricity ceases in a given material above a characteristic temperature, called its Curie temperature, because the heat agitates the dipoles sufficiently to overcome the forces that spontaneously align them [6].

FE materials exhibit a wide spectrum of functional properties, including switchable polarization, piezoelectricity, high nonlinear optical activity, pyroelectricity, and nonlinear dielectric behavior [8].

These properties are crucial for ap-plication in electronic devices such as high-dielectric-constant capacitors, pyroelectric devices, transducers for medical diagnostic, piezoelectric sound navigation and ranging (sonars), electro-optic light valves, electromechanical transducers, sensors, micro actuators, infrared (IR) detectors, microwave phase filters, and nonvolatile memories [9].

This unique combination of properties of FE materials has attracted researchers and engineers for a long time. Over the past few years, the ferroelectricity at nanoscale received a great attention from the scientists on the development of new technologies. The demand for FE systems with specific

* Correspondence: harith.m.s.h@gmail.com

applications enforced the in-depth research in addition to the improvement of processing and characterization techniques [9],[10].

2. Perovskites

Perovskites are a class of materials with a specific type of crystal structure, which is characterized by a repeating pattern of atoms arranged in a particular way. The name "perovskite" comes from the mineral called perovskite, which was first discovered in the Ural Mountains in Russia in the 19th century. The mineral was named after the Russian mineralogist Lev Perovski [11],[12].

Perovskite materials have a cubic crystal structure, with a repeating pattern of atoms arranged in a specific way. The crystal structure consists of a small cation (positively charged ion) surrounded by an anion (negatively charged ion) in a cubic arrangement. The cation is typically a transition metal, such as titanium or nickel, and the anion is typically oxygen [13].

Perovskite materials have a number of unique properties that make them at-tractive for a variety of applications. For example, they have a high electrical conductivity, which makes them useful in electronic devices such as transistors and solar cells. They also have a high dielectric constant, which makes them useful in capacitors and other electronic components [14].

Perovskite solar cells are a type of solar cell that uses perovskite materials as the light-absorbing layer. These solar cells have the potential to be more efficient and less expensive to produce than traditional silicon-based solar cells. They have shown promising results in laboratory tests and are beginning to be commercialized [15].

Perovskite materials have also been explored for use in LED lights, lasers, and other optoelectronic devices. They have the potential to be more efficient and less ex-pensive to produce than traditional materials used in these applications [16].

3. Preparation and Phase Diagram

A ternary phase diagram is a graphical representation of the phase behavior of a system consisting of three components. It is a useful tool for understanding the phase behavior of systems containing three components, such as alloys, polymer blends, and chemical systems. The three components are represented by the corners of a triangle, with the amount of each component represented by the distance from the corner to the center of the triangle. The center of the triangle represents the point at which all three components are present in equal amounts.

Phase boundaries on a ternary phase diagram are lines that represent the conditions under which two phases can coexist. For example, the line separating the sol-id and liquid phases represents the melting point of the system. The line separating the liquid and gas phases represents the boiling point of the system.

Ternary phase diagrams can be used to predict the properties of a system at different compositions and temperatures. They can also be useful for understanding the phase behavior of systems with complex phase diagrams, such as systems with multiple solid phases or liquid-liquid phase separation.

In addition to showing the phase boundaries, ternary phase diagrams can also in-clued lines that represent the compositions of specific phases, such as the composition of a particular solid phase or the composition at which a liquid phase be-comes unstable.

Ternary phase diagrams can be constructed using experimental data or by using computational models to predict the phase behavior of a system. They can be useful for a variety of applications, including the development of new materials and the optimization of processes in the chemical and materials industries.

Now after Now, after placing the components and raw materials on the three-phase triangle, and after making the special equation, a new compound with a new ferroelectric perovskite phase was put forward by means of the trinary-phase diagram.

After that, the materials were mixed using the solid-state reaction method using a mortar for more than three hours of grinding today for the mixed materials ac-cording to the concentrations and proportions predicted by the three-phase triangle.

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The following figure shows the three-phase triangle produced using the Origin 2018 program, as it shows that there are three points in a specific area called Morphotropic Phase Boundary (MPB).

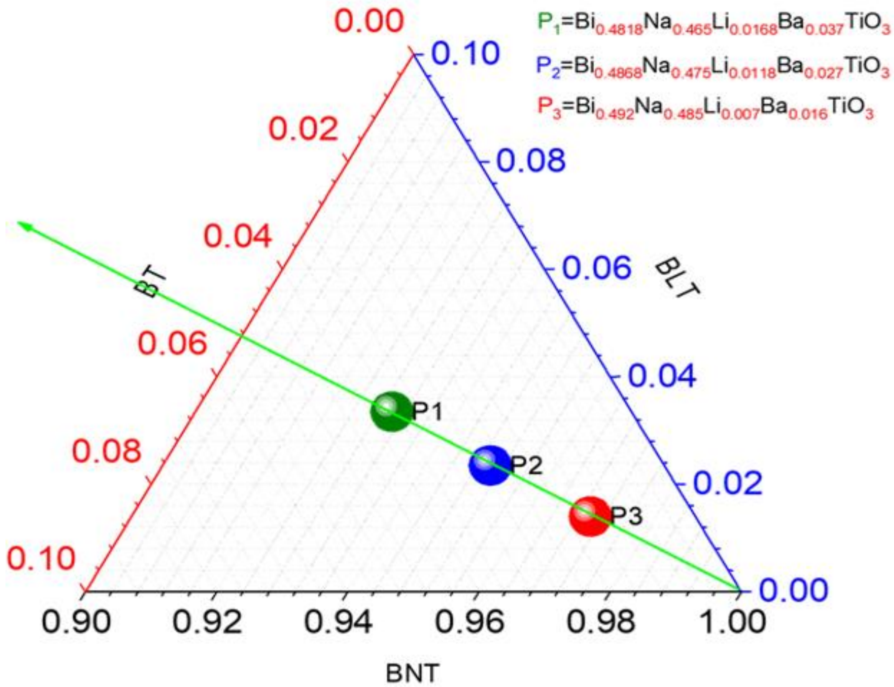

Figure 1.
Ternary phase diagram.

4. Reaction Method

Solid state reaction method was used to prepare new perovskite ferroelectric compound, where many compound are used as source materials like sodium carbonate, bismuth carbonate, lithium nitrate, barium carbonate and titanium oxide.

Three point was taken in a region inside phase diagram called morphotropic phase boundary region (MPB), the point one was ($Bi_{0.48175}$ $Na_{0.465}$ $Li_{0.001675}$ $Ba_{0.0365}$ Tio_3), point two was ($Bi_{0.48675}$ $Na_{0.475}$ $Li_{0.01175}$ $Ba_{0.0265}$ Tio_3) and point three was ($Bi_{0.492}$ $Na_{0.485}$ $Li_{0.007}$ $Ba_{0.016}$ Tio_3).

5. Morphotropic Phase Boundary (MPB)

Morphotropic phase boundary (MPB) is a term used to describe the boundary be-tween two phases or regions in a material that exhibits a change in crystal structure as a function of composition. MPBs are often found in piezoelectric materials, which are materials that can convert mechanical stress into an electrical voltage and vice versa. These materials are of great importance in a variety of technological applications such as sensors, actuators, and transducers [17],[18].

One important aspect of MPBs is that they can give rise to enhanced piezoelectric properties, which makes them attractive for use in various applications. For example, in the case of bismuth lithium titanate (BLT), an important piezoelectric material, the MPB occurs at a specific composition where the material exhibits the highest piezoelectric coefficient. This makes it possible to tailor the piezoelectric properties of the material by adjusting its composition to be close to the MPB [18].

6. Calcination, Pressing and Sintering Process

After mixing the row materials by using solid state reaction method then now must by objected to heat treatment under high temperature reached to 750 °C degree for many hours, where this process called the calcination process, by using thermal furane in the laboratory starting from the laboratory temperature raising to 750 °C degree for three hours to reach to this temperature and now it's It has been stabilized to 750 °C for three hours and finally now returns to laboratory temp. for three hours. This process is very important process to obtain the phase of matter.

After that then pressing this powder under 4 tons for 5 min to obtain on hard pallet to examinate the other measurements on this matter. Finally, after pressing the matter must me now objected to another high more heat treatment reached to 1000 °C to get on high dense pallet.

7. X- Ray Diffraction Analysis

X-ray diffraction (XRD) is a powerful analytical technique that is used to identify the crystal structure of a material. It is based on the scattering of X-rays by the atoms in a crystal, and the resulting diffraction pattern can be used to identify the crystal structure and the chemical composition of the material.

XRD has a wide range of applications, including the identification of minerals, the characterization of materials for use in the semiconductor industry, and the analysis of pharmaceuticals.

The basic principle of XRD is that when X-rays are incident on a crystal, they are scattered in a pattern that is characteristic of the crystal structure. The diffraction pattern is the result of the constructive and destructive interference of the scattered X-rays, and it is this pattern that is used to identify the crystal structure. In this research in this research, the three samples prepared by the solid-state method were examined, as shown in the following figures.

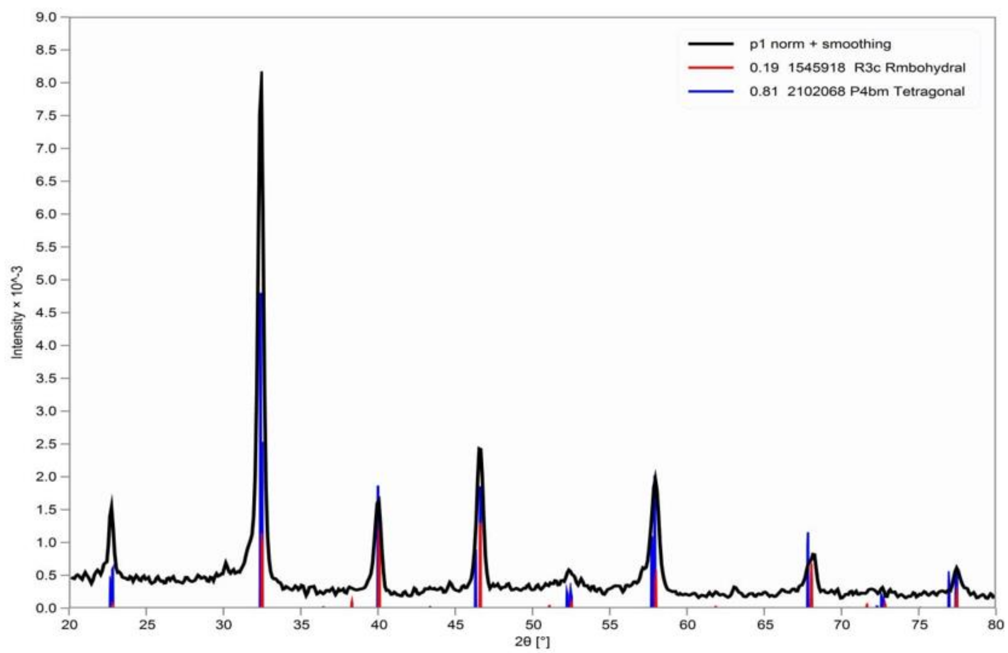

Figure 2.
1st Point XRD diffraction.

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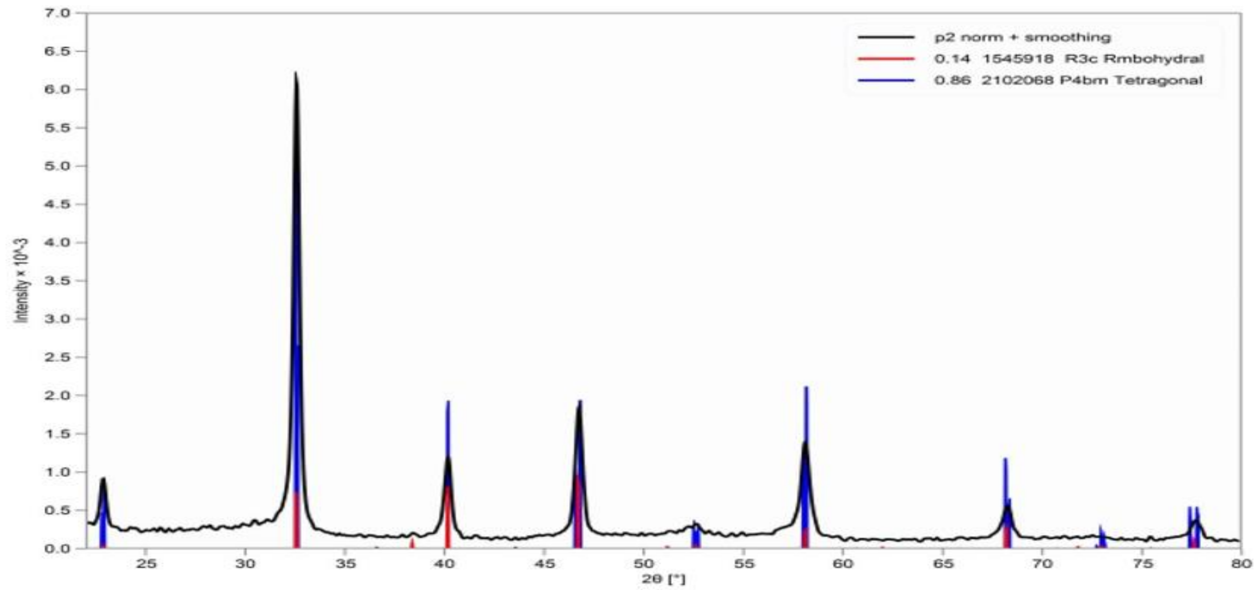

Figure 3.
2nd Point XRD diffraction.

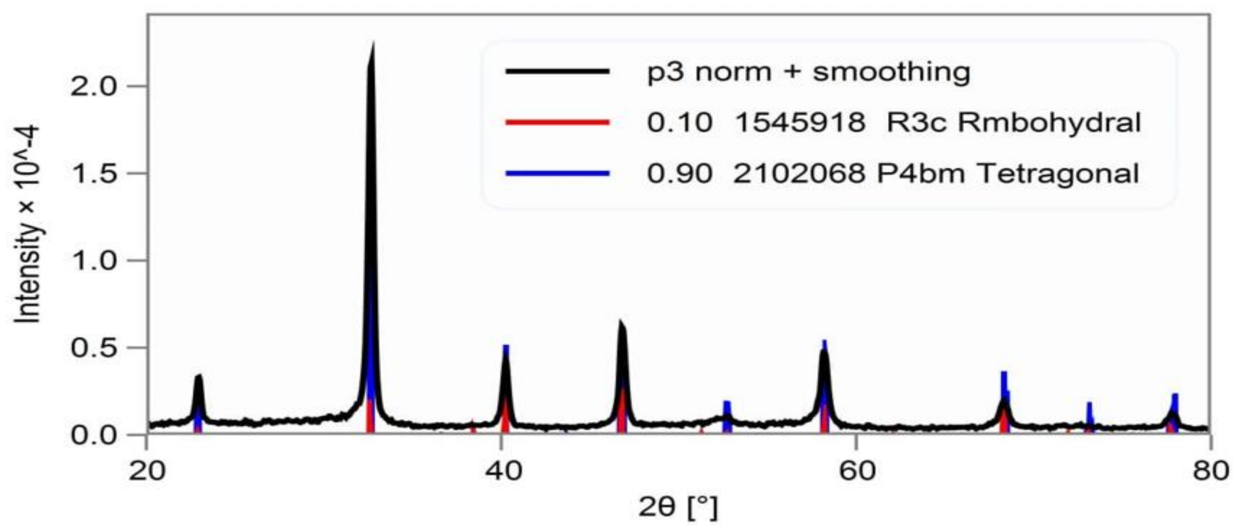

Figure 4.
3rd Point XRD diffraction.

Figure 2,3,4 Show the X-ray Diffraction exam of the three points pointers on the Ternary phase diagram shows in figure 1 in the Morphotropic phase boundary region where these graphs expressed the miller induces and Bravies lattice structure (Tetragonal Bravies lattice) where from x -ray diffraction analysis its appears that the lattice constant (a=b≠c) and the angles its equals according to the XRD exam.

8. SEM and EDX Analysis

8.1. Scanning Electron Microscopy (SEM):

SEM is a powerful imaging technique used to obtain high-resolution images of the surface of a sample.

It works by scanning a focused electron beam across the specimen, and the interaction between the electrons and the sample generates various signals, which are then detected to form an image. SEM provides detailed information about the sample's morphology, topography, and composition. It is widely used in materials science, nanotechnology, biology, geology, and many other fields [19],[20].

Some key features and uses of SEM analysis include:

- High-resolution imaging of surfaces at magnifications ranging from 10x to over 300,000x.
- 3D imaging capability, providing depth information about the surface features.
- Detailed analysis of microstructures, particle size, and distribution.
- Characterization of fractures, wear patterns, and material defects.
- Identification of elemental composition through secondary electron (SE) and backscattered electron (BSE) imaging [21].

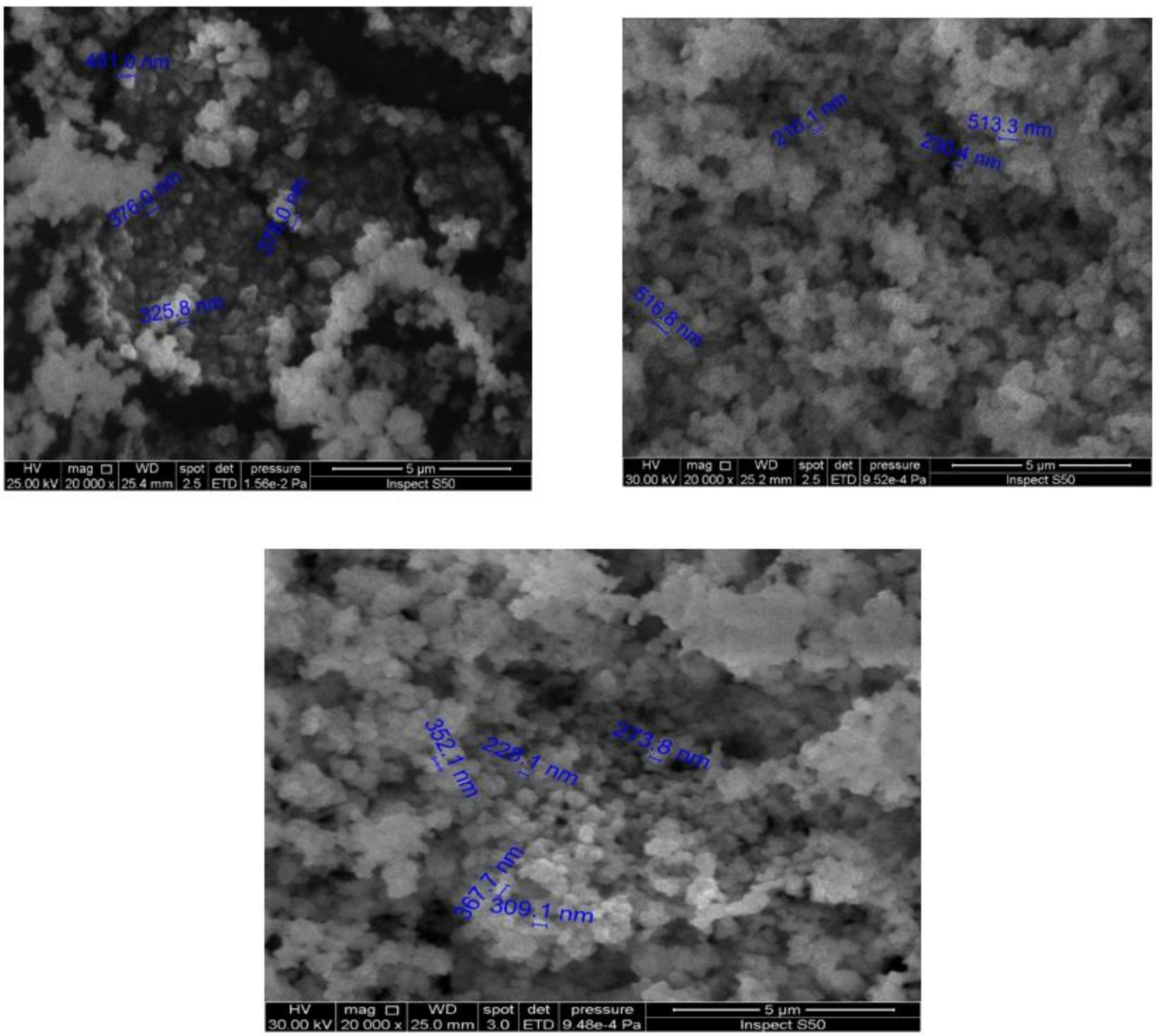

Figure 5.
Show SEM of Point one, Point Two and point three of new ferroelectric materials.

8.2. Energy Dispersive X-ray Spectroscopy (EDX)

EDX is an analytical technique that complements SEM by providing information about the elemental composition of a sample. When the electron beam interacts with the sample, it induces the emission of characteristic X-rays from the atoms present in the sample. These X-rays are collected and analyzed using an energy-dispersive detector, allowing for the identification and quantification of elements present in the sample [21], [22].

8.2.1. Key Aspects of EDX Analysis Include

- Elemental analysis of materials, identifying major and trace elements.
- Elemental mapping, showing the spatial distribution of elements on the sample's surface.
- Quantitative analysis of elemental composition, usually reported as weight percentages.
- Non-destructive analysis, which means samples can be examined without significant alteration.

8.2.2. Combined SEM-EDX Analysis

The combination of SEM and EDX provides comprehensive information about the surface morphology and elemental composition of a sample. Researchers and scientists often use both techniques together to gain a better understanding of the material's structure and properties. For instance, after identifying specific surface features using SEM imaging, they can use EDX to determine the chemical composition of those features [22].

Overall, SEM-EDX analysis is a valuable tool in materials characterization, failure analysis, and research across various scientific and industrial disciplines. It helps researchers make informed decisions and draw conclusions based on both the physical structure and the elemental makeup of the samples they study [23].

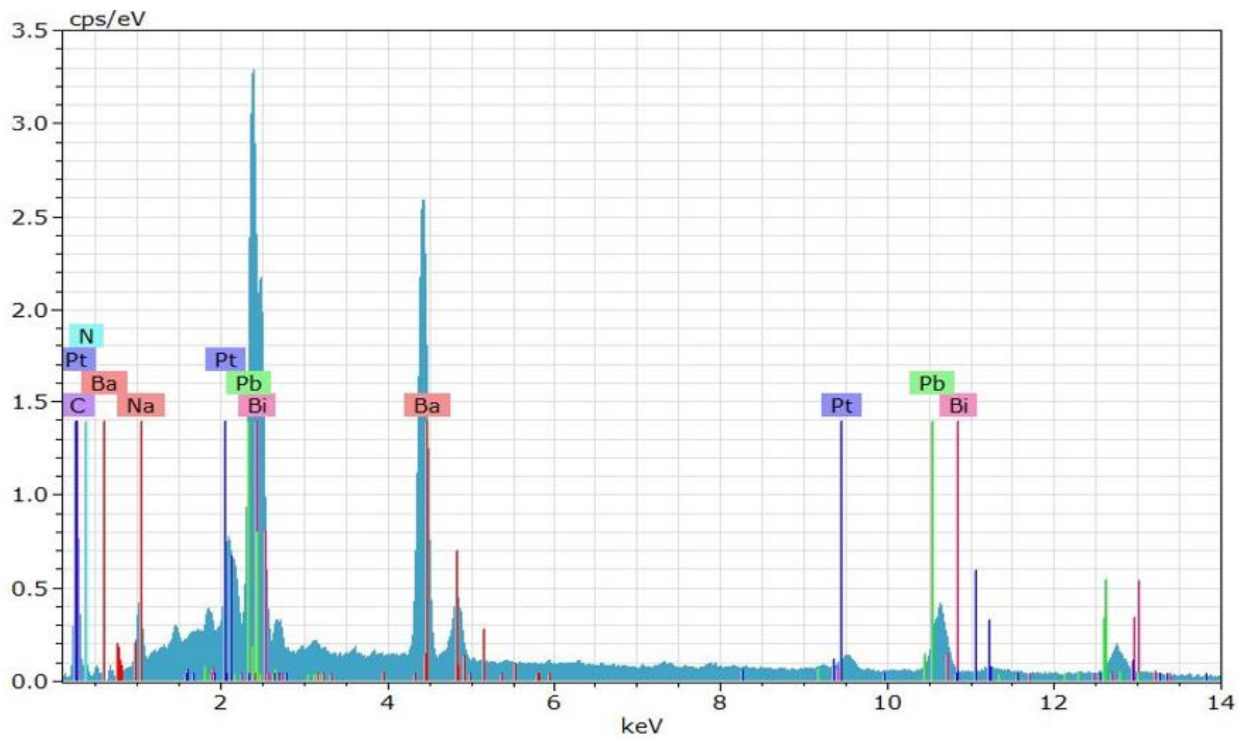

Figure 6.
Show the EDX surface micrograph of point one of new ferroelectric compound.

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Table 1.
Show the EDX determinations of point one of new ferroelectric compound.

Element	Wt %	Wt % Sigma	Norm Wt %
Barium	39.29297	1.176534	16.06
Lead	26.242	1.001	7.11
Carbon	14.5616	3.182	68.06
Bismuth	6.664114	0.422	17903
Platinum	3.841133	0.25	1.105
Sodium	2.400344	0.25	5.86
Total	93.002	-	100

9. Conclusion

In this research, a new ferroelectric compound with a perovskite phase was prepared from several basic materials by mixing them using the solid-state reaction method, where the heat treatment process was carried out to high temperatures of up to 750 degrees Celsius, and then the samples resulting from the X-ray diffraction method were examined. A new ferroelectric phase perovskite. The main components were mixed based on the three-phase diagram to know the ratios and concentrations at which the compound is prepared.

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