International Journal of Nanoelectronics and Materials
IJNeaM
ISSN 1985-5761 | E-ISSN 2232-1535

Crystal properties analysis using the Cramer-Cohen method and the MAUD software in $SrTiO_3$ ceramic doped with ruthenium oxide (RuO_2)

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Received 20 December 2024, Revised 24 September 2025, Accepted 8 October 2025

ABSTRACT

The analysis of Strontium Titanate ($SrTiO_3$) ceramics doped with Ruthenium (Ru) with variations of dopant concentration at 0%, 0.5%, and 1% using the Solid-State Reaction method was successfully executed. The annealing process started at room temperature and was raised to an annealing temperature of 850°C at a heating rate of 1.67°C/minute, held constant for 8 hours, and then cooled down to room temperature for approximately 13 hours. XRD data analysis using the Cramer-Cohen method showed lattice parameters of a = b = c = 3.905 Å for undoped $SrTiO_3$, a = b = c = 3.903 Å for $SrTiO_3$ doped with 0.5% Ruthenium, and a = b = c = 3.901 Å for $SrTiO_3$ doped with 1% Ruthenium, with a cubic crystal structure. XRD data analysis using the MAUD software employing the Rietveld method with 21 iterations resulted in the diffraction pattern of SrTiO3 ceramics, yielding lattice parameters of a = b = c = 3.907 Å for undoped $SrTiO_3$, a = b = c = 3.906 Å for $SrTiO_3$ doped with 0.5% Ruthenium, and a = b = c = 3.905 Å for $SrTiO_3$ doped with 1% Ruthenium, with a cubic crystal too. The XRD data analysis using both the Cramer-Cohen method and the MAUD software employing the Rietveld method showed relatively close lattice parameters, indicating that the experimental XRD spectra closely align with the theoretical analysis performed by the MAUD software.

Keywords: *Crystal properties analysis, Cramer-Cohen method, MAUD software, $SrTiO_3$, Ceramic*

1. INTRODUCTION

Over the past few decades, there has been a marked and sustained increase in the utilization and exploration of ferroelectric materials across a broad spectrum of scientific and technological disciplines. This surge in interest can be attributed to the remarkable multifunctionality exhibited by these materials, which include spontaneous electric polarization—commonly referred to as ferroelectricity—that can be reversed by the application of an external electric field. In addition to their intrinsic ferroelectric properties, many of these materials demonstrate a unique combination of electrical conductivity and semiconducting behavior, which can be modulated through structural modifications, external stimuli, or compositional tuning. These versatile electrical and structural characteristics have positioned ferroelectric materials at the forefront of next-generation device development, particularly in areas such as non-volatile ferroelectric random-access memory (FeRAM), piezoelectric sensors, energy harvesting systems, microelectromechanical systems (MEMS), and novel nanoelectronic architectures. As research continues to unveil new mechanisms and enhance material performance, ferroelectrics are increasingly regarded as a key component in the advancement of multifunctional and energy-efficient electronic systems [1].

2. THEORETICAL BACKGROUND

Strontium Titanate ($SrTiO_3$) is a ferroelectric material that has a cubic perovskite structure that falls under the category of metal oxide materials. It exhibits good conductivity, paraelectricity, and photocatalysis properties, as well as environment-friendly and affordable [2]. Its cubic structure consists of a titanium atom in the centre, eight strontium atoms at each corner of the cube, and six oxygen atoms at each wall of the cube, as can be seen in Figure 1 [3].

To enhance and modify the "already great" properties of $SrTiO_3$, we used Ruthenium oxide (RuO_2) as a dopant. Using the Solid-State Reaction method, we successfully integrated $SrTiO_3$ with RuO_2. The already integrated materials then

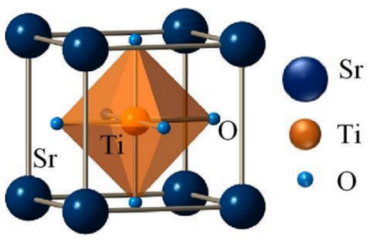


Figure 1. Cubic perovskite structure of $SrTiO_3$ [3]

undergo an annealing process at high temperatures. These processes can be mapped in the following Figure 2.

Figure 3 shows the annealing process. The already homogeneous materials were compacted using the high-temperature annealing process [5].

The addition of dopants affects the lattice structure of the material according to the ionic radius. Dopants with a higher ion radius will shift the peak to the left, while if the ion radius is lower, the shift will be to the right. Both shifts have a lower angle than the peaks without any dopants added [6]. In this study, we used three different dopant variations that is RuO_2, 0%, 0.5%, and 1% concentration. We then analysed the crystal properties analysis was performed using the XRD (X-ray diffraction) using both the Cramer-Cohen Method and the MAUD's Rietveld Methods. Figure 4 shows the effects of ion radius size on the shift of peaks and angles [6].

3. METHODOLOGY

$SrTiO_3$ and RuO_2 powder were measured using a scale and mixed in the mortar. The samples were mixed for two hours to achieve an even mixture. Each composition of the sample can be seen in the Table 1.

The annealing process was carried out after the materials had been mashed together, stated in Figure 3. With a pace of 1.67°C per minute, the temperature was ramped up until it reached 850°C. Then the temperature was held for 8 hours, and it took 13 hours for the samples to reach room temperature again.

Lastly, XRD characterizations were carried out. We used both the theoretical approach, MAUD (Material Analysis Using Diffraction) software, and the experimental Cramer-Cohen (XRD-Spectra) approach. This will allow more comprehensive analysis and cross, and validated results of analysis to be obtained.

XRD works by shooting X-ray beams into the materials that will be observed. When the beam interacts with the material, absorption, diffraction, or fluorescence can happen. These processes could help us identify and determine the parameters of the lattice structure and particle size, which ultimately helps us determine the crystalline phase in the materials afterward [7–10].

4. DISCUSSION AND RESULTS

4.1. Cramer-Cohen XRD Data Analysis

Using the X-ray diffractometer, with an incoming angle of 2θ, an angle range of 20–80°, and an interval of 0.02°/minute, we successfully analysed the lattice parameter and the crystal structure of $SrTiO_3$ doped with RuO2. Table 2 shows the comparison between our calculation and the existing literature.

Figure 5 (a), (b), and (c) illustrate the intensity vs 2θ graphs for RuO_2-doped $SrTiO_3$ at 0%, 0.5%, and 1%, respectively.

Table 1. Sample composition

Dopant (%)	Strontium titanate (g)	Titanium oxide (g)	Ruthenium oxide (g)
0	1.2000	0	0
0.5	1.1940	0.0060	0.0060
1	1.1880	0.0120	0.0120

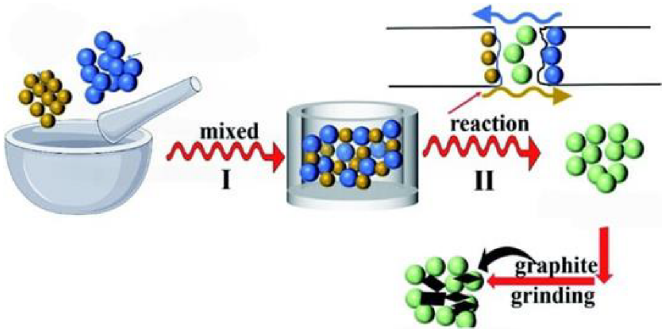


Figure 2. Solid-State Reaction method. $SrTiO_3$ and RuO_2 were mixed and grinded using mortar and pestle until they became homogeneous, which then followed by compaction [4]

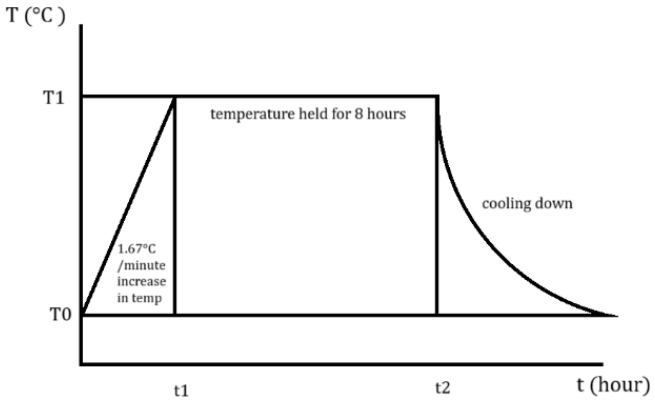


Figure 3. The annealing process. The already homogeneous materials were compacted using the high-temperature annealing process [5]

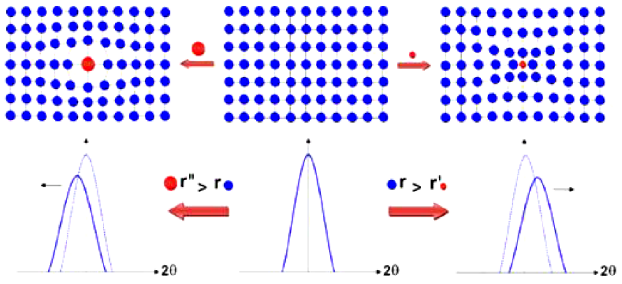


Figure 4. The effects of ion radius size on the shift of peaks and angles [6]

From these graphs, diffraction peaks corresponding to the Miller index (hkl) of the unit cell were observed. The obtained peaks represent the distribution of the crystalline orientations. The diffraction peaks can be assigned to the Miller index from which the lattice parameters can be determined. In this research, the method of Cramer-Cohen was used in determining the lattice parameters by matching the observed diffraction peaks in the graphs with the ICDD literature for $SrTiO_3$ to ascertain the hkl values. Thus, the

calculated lattice parameters are compared with the ICDD data to evaluate the influence of the added RuO_2 dopant on the $SrTiO_3$ ceramics.

Table 2 shows obtained lattice parameter of $SrTiO_3$ ceramics.

The lattice parameters of the various doping calculated by the Cramer-Cohen method are close and similar to that of the ICDD lattice parameters. The lattice parameters of $SrTiO_3$ ceramics doped with RuO_2 at 1% determined were 3.901 Å, while for 0 is 3.905 Å, and for 0.5% is 3.903 Å. It can be observed that the lattice parameter decreases upon the increase in the dopant concentration. The reduction is due to the effect of the dopant having a different ionic radius than that of the parent material. Due to the smaller ionic radius, Ru ions replace the Ti ions, which resulted in the reduced lattice parameter of the doped $SrTiO_3$ compared to that of the pure material [6]. Figure 5 presents the intensity against 2θ graph for different doping concentrations of $SrTiO_3$-RuO_2 ceramics.

4.2. MAUD Data Analysis

The MAUD software analysis of XRD data was performed using the Rietveld method, using 21 iterations. In such a way, the refinement in the diffraction pattern of $SrTiO_3$ doped with RuO_2 ceramics was developed. Figure 6 shows diffraction pattern of $SrTiO_3$ ceramics obtained from MAUD software (a) 0%, (b) 0.5%, (c) 1%.

Table 2. Obtained lattice parameter of $SrTiO_3$ ceramics

Doping variations (%)	Lattice parameter (Å)	Lattice parameter ICDD (Å) [11]
	a = b = c	a = b = c
0	3.905	3.905
0.5	3.903	-
1	3.901	-

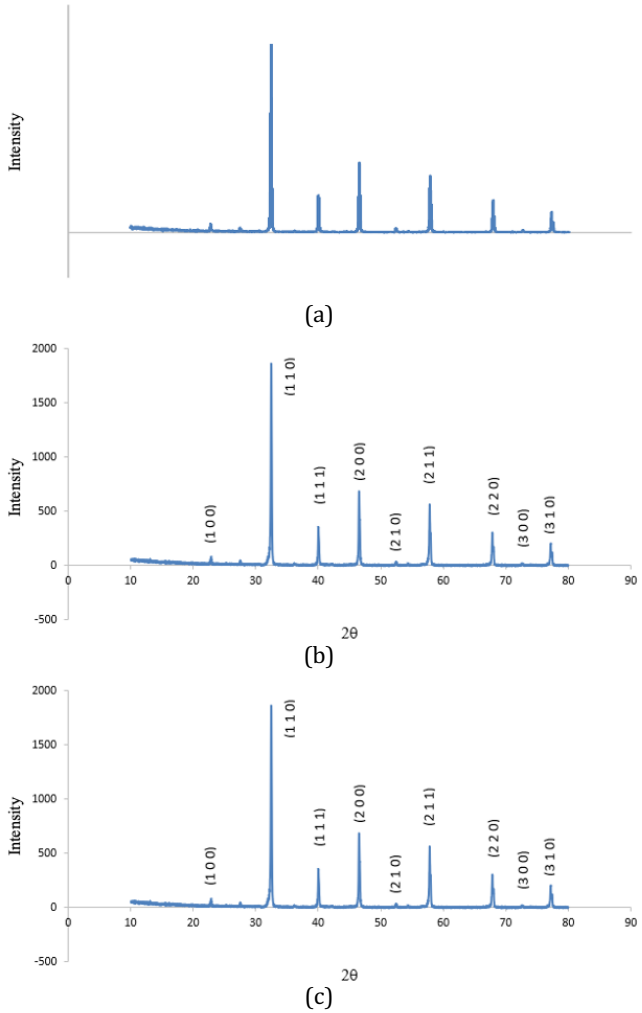


Figure 5. Relation of 2θ (a) without dopant, (b) with 0.5% dopant, and (c) with 1% dopant

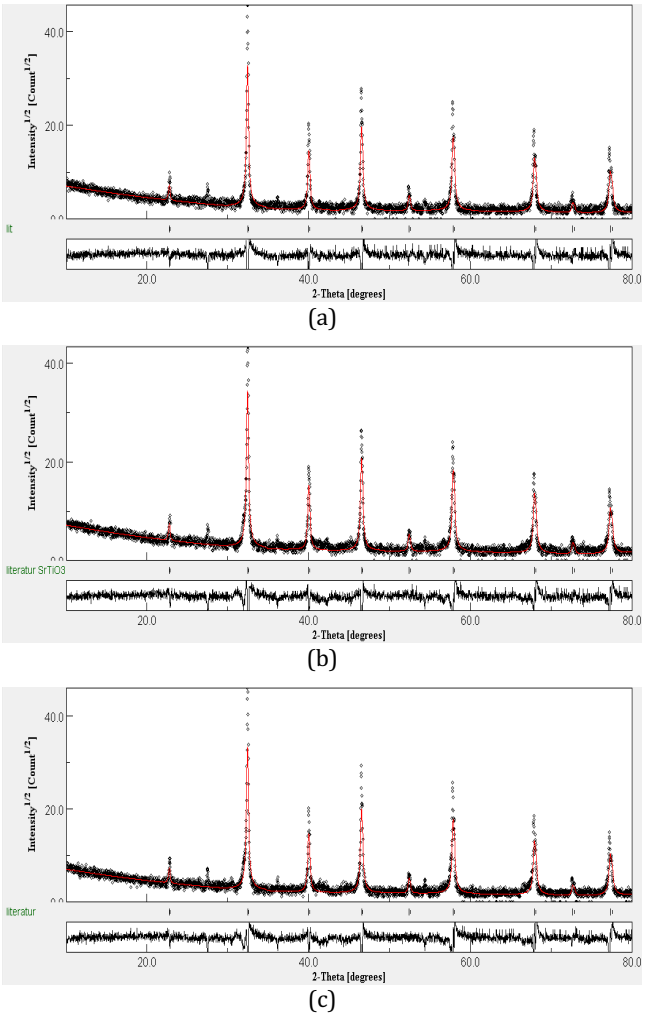


Figure 6. Diffraction pattern of $SrTiO_3$ ceramics obtained from MAUD software. (a) 0%, (b) 0.5%, and (c) 1%

The resulting XRD was processed using MAUD software to determine the crystal size in each phase of $SrTiO_3$ using Equations (1), (2), (3):

$$\Sigma\alpha sin^2\theta = C\Sigma\alpha^2 + B\Sigma\alpha\gamma + A\Sigma\alpha\delta \quad (1)$$

$$\Sigma\gamma sin^2\theta = C\Sigma\alpha\gamma + B\Sigma\gamma^2 + A\Sigma\gamma\delta \quad (2)$$

$$\Sigma\delta sin^2\theta = C\Sigma\alpha\delta + B\Sigma\gamma\delta + A\Sigma\delta^2 \quad (3)$$

Table 3 shows obtained lattice parameter of RuO_2-doped $SrTiO_3$ ceramics using the MAUD software.

The lattice parameters that were obtaine from the MAUD software analysis are also similar to the ICDD literature values, and showed a decreased trend, without showing any significant difference among the analysed samples. This can occur because the dopants are in small concentration and with the addition that the MAUD software has the possibility of iteration(s) that does not run smoothly. Figure 7 shows $SrTiO_3$ ceramic structure using MAUD, (a) 0%, (b) 0.5%, (c) 1%. MAUD software that the $SrTiO_3$ with RuO_2 dopant has a cubic structure.

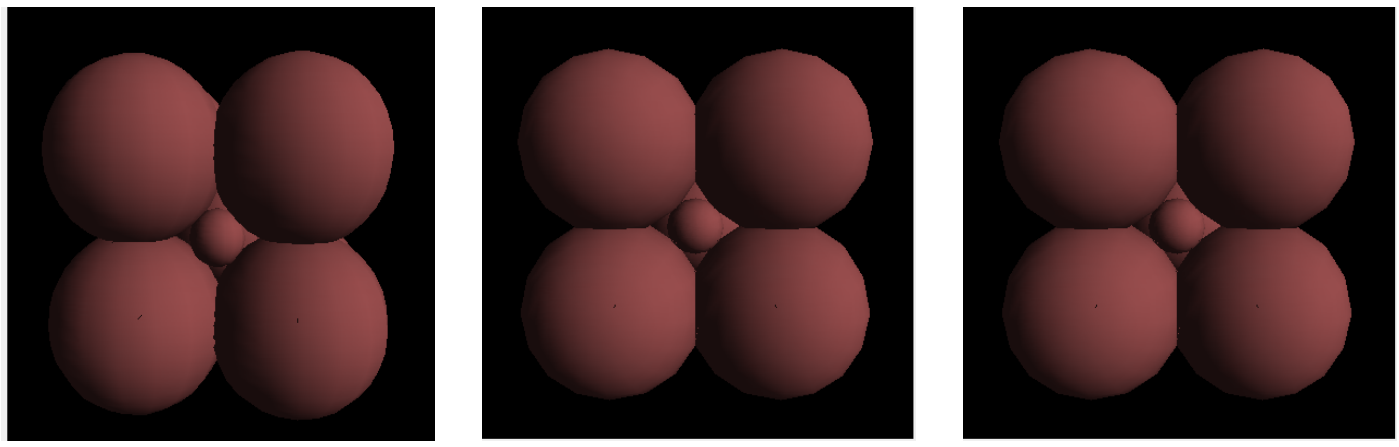
Figure 7 presents the images of $SrTiO_3$ samples with varying Ruthenium dopant concentrations of 0%, 0.5%, and 1%. As observed, there are no clearly distinguishable differences among the samples in terms of their visual diffraction patterns. This lack of observable variation can be attributed to the extremely small changes in the lattice parameters, which are on the order of approximately 0.002 Å (0.2 picometers). Such minimal shifts fall well below the resolution limit of the MAUD software used for structural analysis, rendering them undetectable through visual inspection of the diffraction data. Therefore, while slight structural modifications may indeed be present due to doping, they are too subtle to be captured or distinguished by this analytical approach alone.

5. CONCLUSION

Analysis of crystalline properties of ceramic $SrTiO_3$ doped by RuO_2 with several doping variation (0%, 0.5%, 1%) was successfully conducted using The Solid-State Reaction method. The $SrTiO_3$ lattice parameter obtained from the Cramer-Cohen method were 3.905 Å for 0% dopant concentration, 3.903 Å for 0.5% dopant concentration, and 3.901 Å for 1% dopant concentration. The $SrTiO_3$ lattice parameter obtained from the MAUD method were 3.907 Å for 0% dopant concentration, 3.906 Å for 0.5% dopant concentration, and 3.905 Å for 1% dopant concentration. From the obtained data, it can be concluded that the addition of RuO_2 dopant results in lattice parameter values that shrink as the concentration of the doping increases. This happens due to the smaller ionic radius of Ru dopant, resulted in that that smaller Ru ions replace the Ti ions in the $SrTiO_3$. This phenomenon reduced the lattice parameter compared to that of the pure $SrTiO_3$. The results of XRD analysis show the structure of $SrTiO_3$ in cubic form. It also can be concluded that the data that were obtained from Cramer-Cohen method and the MAUD method yields a similar result, indicating that the experimental XRD spectra closely align with the theoretical analysis performed by the MAUD software.

Table 3. Obtained lattice parameter of RuO_2-doped $SrTiO_3$ ceramics using the MAUD software

Doping variations (%)	Lattice parameter (MAUD) (Å)	Lattice parameter ICDD (Å) [11]
	a = b = c	a = b = c
0	3.907	3.905
0.5	3.906	-
1	3.905	-



(a) (b) (c)

Figure 7. $SrTiO_3$ ceramic structure using MAUD, (a) 0%, (b) 0.5%, and (c) 1%. MAUD software that the that the $SrTiO_3$ with RuO_2 dopant has a cubic structure

ACKNOWLEDGMENTS

This research was supported by Hibah Penelitian grant from Direktorat Jendral Pendidikan Tinggi, Riset dan Teknologi, Kementerian Pedidikan, Kebudayaan, Riset dan Teknologi of Republic of Indonesia with contract number: 22346/IT3.D10/PT.01.03/P/B/2024 and 027/E5/P6.02. 00PL/2024 dated June 12, 2024.

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