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Comparative X-Ray Diffraction Analysis of Quartz Samples for Crystallographic and Phase Composition Variations

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Abstract: ***This research compares two quartz rock samples using X-ray powder diffraction to evaluate differences in their crystal structure and mineral composition. Each powdered sample was analyzed using a Philips X'Pert Pro diffractometer. The analysis revealed that Sample 1 consists entirely of quartz with a hexagonal crystal structure and space group $P3_12_1$, while Sample 2 contains quartz (21.9%), anorthite (53.9%), and muscovite (24.2%), crystallizing in mixed hexagonal and anorthic systems. Minor variations in lattice parameters were observed, attributed to secondary mineral inclusions in Sample 2. The study confirms the effectiveness of XRD in identifying phase composition and crystallographic features of quartz samples. The aim of this study is to compare the crystallographic and mineralogical compositions of two quartz rock samples using X-ray powder diffraction.***

Keywords: X-ray diffraction, quartz, crystalline structure, mineral analysis, phase composition

1. Introduction

The quartz, is one of the commonest of all rock forming minerals and one af the most important constituents of the earth's crust. Chemically, it is silicon dioxide, also known as silica, is a chemical compound that is ar axide of silicon with the chemical formula SiO,. It has been known since ancien times. Silica is most commonly found in nature as sand or quartz, as well as in the cell walls of diatoms [1].

Silica is manufactured in several forms including fused quartz, crystal fumed silica (or pyrogenic silica), colloidal silica, silica gel, Silica is used primarily in the production of glass for windows, drinking glasses, beverage bottles, and many other uses. The majority of optical fibers for telecommunications are also made from silica. It is a primary raw material for many ceramics such as earthenware, stoneware, and porcelain [2].

Silica is a common additive in the production of foods, where it is used primarily as a flow agent in powdered foods, or to absorb water in hygroscopic applications[3]. It is the primary component of diatomaceous earth, which has many uses ranging from filtration to insect control. It is also the primary component of rice husk ash, which is used, for example, in filtration and cement manufacturing [4,5].

Silica thin films grown on silicon wafers through thermal oxidation serve as effective electrical insulators in microelectronies, where they act as electric insulators with high chemical stability. In electrical applications, it can protect the silicon.

Understanding the mineralogical variations and crystal structures of quartz samples enhances applications in materials science, geological mapping, and industrial quality contro

2. Methodology

The sample was mechanically milled for 30 s to obtain a homogeneous powder, which was then analyzed using X-ray diffraction. When the incident X-rays satisfy Bragg's condition, constructive interference occurs and the diffracted signal is recorded as a count rate. The diffraction patterns (Figures 1 and 2) were collected in step-scan mode using a 2θ range of 0–100°, a step size of 0.03°, and a counting time of 4 s per step. These parameters were selected to obtain a smooth, high-resolution diffractogram

3. Results and Discussion

The X-ray diffraction data obtained for both samples were subjected to smoothing prior to structural analysis using a reference diffraction pattern. This procedure allowed for the extraction of crystallographic information, including unit cell dimensions, space group symmetry, and atomic positional parameters. The diffractogram corresponding to sample 1 is presented in Figure 1 and tables 1 and 2, and reveals the presence of a single crystalline phase, identified as quartz (SiO_2). The diffraction pattern recorded for sample 2 is shown in Figure 2, and tables 3 and 4..

The analysis confirms that the sample 1 is composed exclusively of quartz, whereas the sample 2 consists primarily of quartz with trace amounts of secondary phases, including anorthite and muscovite. Both samples crystallize in a hexagonal structure characteristic of quartz and belong to the same space group ($P3_12_1$).

Minor deviations in lattice parameters, atomic density, and unit cell volume were observed between the two samples. Such variations are attributed to the incorporation of trace impurity phases within the sample 2 lattice, particularly anorthite, which induces slight distortions in the quartz framework

Table 1: Consist of structure data for quartz of sample (1)

Crystal System	Hexagonal
Space Group	$P3_121$
Space Group Number	152
a (A^O) basis vectors	4.912
b(A^O) basis vectors	4.912
c(A^O) basis vectors	5.402
α angle between y, z	90
β angle between x, y	90
γ angle between x, z	120
Calculated Density (g/em^3)	2.65
Volume of cell	112.88
Z	3
RIR	4.44

Table 2: Illustrated the lattice plane, distance (d) and Miller indices (hkl) for quartz in sample (1)

No.	h	k	l	d (A^O)	2theta (deg)	I %
1	0	1	0	4.25392	20.865	19.3
2	1	1	0	3.34208	26.651	100
3	0	1	1	2.45600	36.557	6.6
4	2	1	0	2.28019	39.488	7.4
5	1	1	1	2.2357	40.307	3.5
6	0	2	0	2.12696	42.466	5.3
7	1	2	0	1.97908	45.812	2.8
8	2	1	1	1.8191	50.164	12.3
9	3	0	0	1.80067	50.654	0.3
10	2	2	0	1.67104	54.900	3.8
11	3	1	0	1.65822	55.360	1.6
12	0	2	1	1.60683	57.252	0.2
13	1	2	1	1.54102	59.982	9.1
14	3	1	1	1.45218	64.071	1.8
15	0	3	0	1.41797	64.071	0.4
16	2	2	1	1.38158	67.773	5.7
17	3	2	0	1.37431	68.181	6.6
18	1	3	0	1.37151	68.339	4.1
19	4	1	0	1.28719	73.516	2.3
20	2	3	0	1.25548	75.693	2.8
21	0	2	2	1.22800	77.677	1.4
22	3	2	1	1.9931	79.925	2.8
23	1	2	2	1.19745	80.074	0.8
24	4	1	1	1.18339	81.223	2.5
25	0	3	1	1.17982	81.520	2.8
26	1	3	1	1.15265	83.870	1.8
27	4	2	0	1.14010	85.008	0.2
28	2	2	2	1.11789	87.113	0.0
29	3	3	0	1.11403	87.491	0.4

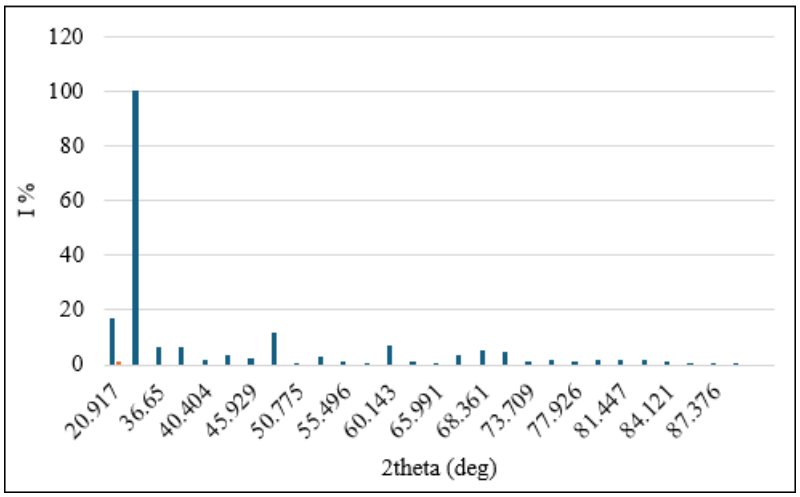

Figure 1: Sticks pattern of the sample (1) shows the intensity and the peak position

Table 3: Fractional coordinates of quartz in sample (1)

No.	Elem.	X	Y	Z	Biso	Sof.	Wyck.
1	O	0.41370	0.14610	0.530193	0.5000	1.0000	6c
2	SI	0.53019	0.00000	0.33333	0.5000	1.0000	3a

Table 4: Consist of structure data for quartz of sample (2)

Mineral Name	Quartz low	Anorthite	Muscovite
Crystal System	Hexagonal	Anorthic	Hexagonal
Space Group	$P3_12_1$	p-l	$P3_22_1$
Space Group Number	154	2	152
a (A^O) basis vectors	4.9000	8.1756	5.2030
b(A^O) basis vectors	4.9000	12.8720	5.2030
c(A^O) basis vectors	5.3900	14.1827	29.9880
α angle between y, z	90	93.1720	90
β angle between x, y	90	115.911	90
γ angle between x, z	120	91.199	120
Calculated Density (g/em^3)	2.67	2.67	2.82
Volume of cell	112.08	1338.75	703.05
Z	3	8	3
RIR	3.12	0.41	--

Table 5: Illustrated the lattice plane, distance (d) and Miller indices (hkl) for quartz in sample (2)

No.	h	k	l	d (A^O)	2theta (deg)	I %
1	1	0	0	4.24352	20.917	17.1
2	0	1	1	3.33420	26.715	100
3	1	1	0	2.45000	36.650	6.7
4	1	0	2	2.74698	39.583	6.5
5	1	1	-1	2.23040	40.404	2.1
6	2	0	0	2.12176	42.575	3.6
7	2	0	1	1.97430	45.929	2.2
8	1	1	-2	1.81285	50.290	11.9
9	0	0	3	1.79667	50.775	0.3
10	0	2	2	1.66710	55.040	2.7
11	0	1	3	1.65448	55.496	1.3
12	1	2	0	1.60390	57.406	0.3
13	2	1	-1	1.53728	60.143	7.3
14	1	1	-3	1.44884	64.236	1.2
15	3	0	0	1.41451	65.991	0.4
16	2	1	-2	1.37828	67.957	3.6
17	2	0	3	1.37113	68.361	5.5
18	0	3	1	1.36818	68.529	5
19	1	0	4	1.28430	73.709	1.3
20	3	0	2	1.25247	75.907	2
21	2	2	0	1.22500	77.926	1.2
22	1	2	-3	1.19650	80.151	1.9
23	1	1	-4	1.18070	81.447	1.7
24	1	3	0	1.17694	81.763	2.1
25	3	1	-1	1.14985	84.121	1.4
26	2	0	4	1.13749	85.249	0.2
27	2	2	-2	1.11520	87.376	0.1
28	3	0	3	1.11140	87.750	0.2

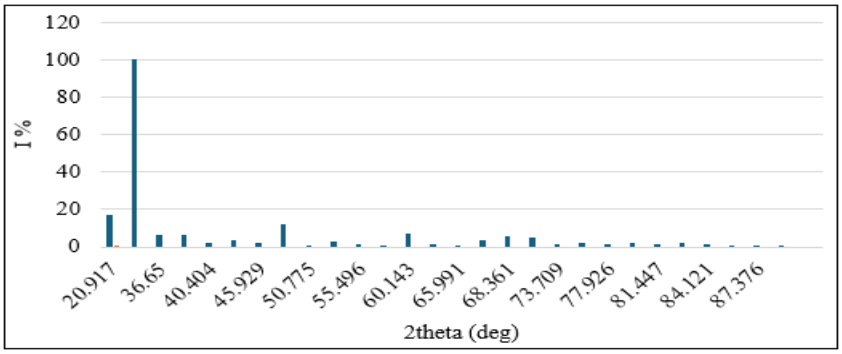

Figure 2: Sticks pattern of the sample (2) shows the intensity and the peak position.

4. Conclusion

The X-ray powder diffraction analysis of the two quartz rock samples showed that the first sample is composed entirely of quartz, while the second sample contains quartz, anorthite, and muscovite. Quartz in both samples exhibits a hexagonal crystal structure, with space groups $P3_12_1$ and $P3_22_1$ for the first and second samples, respectively. The quantitative differences in mineral composition highlight the variation between the two samples, while the crystallographic analysis confirms that quartz is the dominant phase. Overall, the study demonstrates the effectiveness of XRD in identifying and characterizing the crystal structures and phase compositions of rock samples.

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