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Chemical composition and crystal structure of mineral at Amphoe Chiang Khan, Loei Province, Thailand

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ABSTRACT

The powder samples of mineral were prepared by the crush at room temperature and calcination at 600-900°C in air for 3 h. The chemical composition and crystal structure of as crushed and calcined powders were analyzed by X-ray fluorescence spectrometry (XRF) and X-ray diffractometer (XRD). XRF analysis indicated that the oxygen (O), silicon (Si), aluminium (Al), phosphorus (P), calcium (Ca), and sulfur (S) contents of a crushed powder were about 52.160, 32.480, 7.886, 4.466, 1.936, and 1.070%, respectively. Similar analytical results were detected from the calcined powders. The compounds of a crushed powder included the silicon dioxide (SiO₂, 69.490%), aluminium oxide (Al₂O₃, 14.900%), diphosphorus pentoxide (P₂O₅, 10.230%), calcium oxide (CaO, 2.709%), and sulfur trioxide (SO₃, 2.672%). The results showed small differences in the compositions of the calcined powders. These results showed that the mineral are SiO₂-Al₂O₃-P₂O₅-CaO-SO₃ compounds. XRD analysis found that the intensity of (1 7 2), (1 11 1), and (2 8 2) peaks of SiO₂ were relatively large compared to the other peaks. The small peaks observed the planes of CaO and SO₃ while the Al₂O₃ and P₂O₅ are not detected. The XRD results show the traces of SiO₂ phase in the powders, and the monoclinic lattice parameters are less than the reference. These preliminary studies can be used as an important platform for further research. © 2011 Trade Science Inc. - INDIA

KEYWORDS

Chemical composition;
Crystal structure;
X-ray fluorescence;
X-ray diffraction.

INTRODUCTION

A mineral is an element or chemical compound which is naturally occurring and that has been formed as a result of geological processes^[1,2]. An ore has many advantages and important role in the energy and industrial technology. For examples, fossil fuels have been the main energy resources of the world. About 80-90%

of its primary energy needs have been supplied by petroleum oil, natural gas, and coal^[3]. A perlite is composed of 71-75% silicon dioxide or silica (SiO₂), 12.5-18.0% aluminium oxide or alumina (Al₂O₃), 4-5% potassium oxide (K₂O), 1-4% sodium and calcium oxides (Na₂O and CaO), and trace amounts of metal oxides^[4]. This mineral was used in the horticulture, industrial, and construction^[5].

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Thailand has a variety of mineral resources, including tin, tungsten, lead, zinc, lignite, feldspar, kaolin, limestone, and gypsum^[6]. The minerals should be recognized as the non-renewable resources which have limited currently known reserves. This will be economically used. However, the other minerals have been discovered in the natural resources and that can be used to advantages in industrial applications. These are reasons for the growing interest in further study and research.

In this work, we have investigated the mineral at Ban Hua Kaeng, Tambon Hat Sai Khao, Amphoe Chiang Khan, which is located in the northern part of Loei Province, northeastern Thailand. The powder samples were prepared by the crush at room temperature and calcination at 600-900°C in air for 3 hours. The chemical composition and crystal structure are presented.

EXPERIMENTAL

The powder samples of mineral can be prepared by the crush and calcination as summarized in figure 1. The mineral was crushed at room temperature in air it became a powder precursor (sample A). This powder precursor was calcined at 600-900°C in air for 3 hours into the calcined powders (sample B, C, D, and E). The composition of elements and compounds were analyzed by X-ray fluorescence spectrometry (Philips, Magix WDXRF). Phase identification of the powder samples were determined using X-ray diffractometer (Philips, XPert MPD).

RESULTS AND DISCUSSION

The composition of elements and compounds were analyzed by the XRF. The percent compositions are given in TABLE 1 and 2. The XRF analysis revealed the concentrations (%) of all samples which have the same composition. From TABLE 1, the oxygen (O), silicon (Si), aluminium (Al), phosphorus (P), calcium (Ca), and sulfur (S) contents of a powder precursor (sample A) were about 52.160, 32.480, 7.886, 4.466, 1.936, and 1.070%, respectively. Similar analytical results were detected from the calcined powders (sample B, C, D, and E). From TABLE 2, the compounds of a

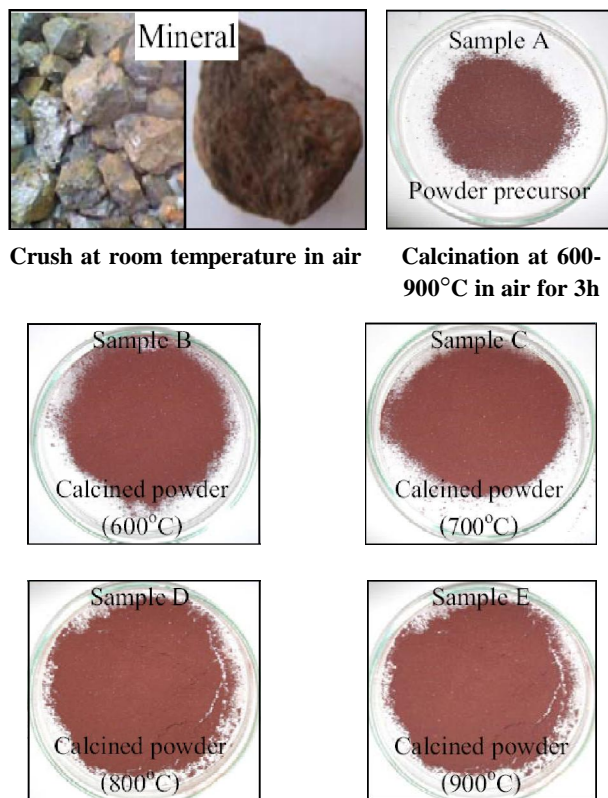


Figure 1 : Fabrication flow chart for the preparation of the powder samples

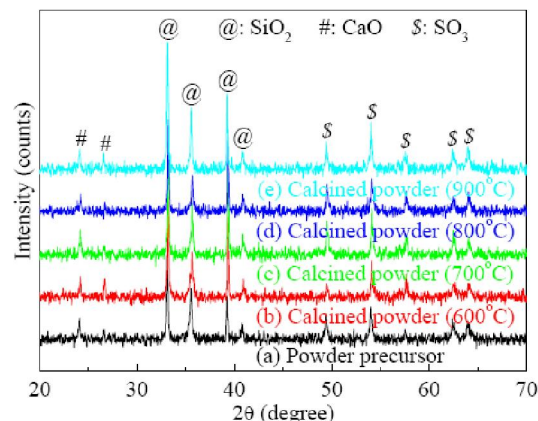


Figure 2 : XRD patterns of the $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-P}_2\text{O}_5\text{-CaO-SO}_3$ compounds

powder precursor (sample A) included the silicon dioxide (SiO_2 , 69.490%), aluminium oxide (Al_2O_3 , 14.900%), diphosphorus pentoxide (P_2O_5 , 10.230%), calcium oxide (CaO , 2.709%), and sulfur trioxide (SO_3 , 2.672%). The results showed small differences in the compositions of the calcined powders (sample B, C, D, and E). These results showed that the SiO_2 , Al_2O_3 , P_2O_5 , CaO , and SO_3 compounds were detected. Hence, it can be expected that the powder samples will

TABLE 1 : Composition of elements obtained from XRF analysis

Elements	Concentrations (%)				
	A(Non)	B(600°C)	C(700°C)	D(800°C)	E(900°C)
Al	7.886	7.315	6.440	6.958	6.516
Ca	1.936	2.788	2.206	2.131	2.816
O	52.160	52.020	52.280	52.080	52.090
P	4.466	5.314	4.895	5.269	5.473
S	1.070	1.218	1.168	<<	1.089
Si	32.480	31.350	33.010	33.560	32.010
Total	99.998	100.005	99.999	99.998	99.994

TABLE 2 : Composition of compounds obtained from XRF analysis

Compounds	Concentrations (%)				
	A(Non)	B(600°C)	C(700°C)	D(800°C)	E(900°C)
Al ₂ O ₃	14.900	13.820	12.170	13.150	12.310
CaO	2.709	3.902	3.086	2.982	3.940
P ₂ O ₅	10.230	12.180	11.220	12.070	12.540
SO ₃	2.672	3.041	2.916	<<	2.721
SiO ₂	69.490	67.060	70.610	71.800	68.490
Total	100.001	100.003	100.002	100.002	100.001

TABLE 3 : Miller indices (hkl) with d-spacing (Å) and 2θ (deg)

2θ (deg)	d-spacing (Å)	Miller indices (h k l)				
		SiO ₂	Al ₂ O ₃	P ₂ O ₅	CaO	SO ₃
24.11	3.6887	-	-	-	(? ? ?)	-
26.59	3.3495	-	-	-	(? ? ?)	-
33.11	2.7034	($\bar{1}$ 7 2)	-	-	-	-
35.59	2.5207	($\bar{1}$ 11 1)	-	-	-	-
39.24	2.2940	(2 8 2)	-	-	-	-
40.85	2.2075	(3 5 2)	-	-	-	-
49.45	1.8417	-	-	-	-	(0 2 2)
54.05	1.6954	-	-	-	-	($\bar{1}$ 2 3)
57.58	1.5994	-	-	-	-	(0 1 5)
62.38	1.4875	-	-	-	-	(0 2 4)
64.03	1.4530	-	-	-	-	(4 0 0)

TABLE 4 : Monoclinic lattice parameters a, b, c, and β of SiO₂ phase

Lattice parameters				Absolute Error
a (nm)	b (nm)	c (nm)	β (deg)	
0.84694	2.73365	0.64155	89.20661	±0.00927
Ref: a=0.9499nm, b=3.0700nm, c=0.7313nm, & β=91.711deg				

contain these species composition. From this point onward, the powder samples will be referred to as SiO₂-

Al₂O₃-P₂O₅-CaO-SO₃ containing.

Phase identification of the SiO₂-Al₂O₃-P₂O₅-CaO-SO₃ compounds (powder samples) were determined using X-ray diffraction at room temperature using CuKα radiation, λ = 0.15406 nm. Each sample was measured in the 2-theta angle range of 20° ≤ 2θ ≤ 70° with scanning rate of 0.02°/sec. The XRD patterns of the powder samples are shown in figure 2. The strong peaks @ can be indexed to the diffraction from the ($\bar{1}$ 7 2), ($\bar{1}$ 11 1), (2 8 2), and (3 5 2) planes of SiO₂ (JCPDS file number 89-7499). The small peaks # is CaO and \$ is SO₃ (JCPDS file number 28-0775 and 73-2169, respectively). For the Al₂O₃ and P₂O₅ are not detected (JCPDS file number 04-0880 and 01-0213, respectively). Miller indices (h k l) with d-spacing (Å) and 2θ (deg) are given in TABLE 3.

The lattice parameters of the samples were calculated from the XRD patterns as shown in TABLE 4. The monoclinic lattice parameters a = 0.8469 nm, b = 2.7336 nm, c = 0.6416 nm, and β = 89.207° were determined from the XRD patterns of the SiO₂ phase. The results showed that the lattice parameters of the powder samples are less than the reference (JCPDS file number 89-7499). The Sherrer calculator determined that the powder samples have crystallite size and lattice strain 88.38±38.08 nm and 0.15%, respectively.

CONCLUSIONS

XRF analysis indicated that the O, Si, Al, P, Ca, and S contents of a crushed powder were about 52.160, 32.480, 7.886, 4.466, 1.936, and 1.070%, respectively. Similar analytical results were detected from the calcined powders. The compounds of a crushed powder included the 69.490% SiO₂, 14.900% Al₂O₃, 10.230% P₂O₅, 2.709% CaO, and 2.672% SO₃. The results showed small differences in the compositions of the calcined powders. These results showed that the mineral are SiO₂-Al₂O₃-P₂O₅-CaO-SO₃ compounds. XRD analysis found that the intensity of ($\bar{1}$ 7 2), ($\bar{1}$ 11 1), and (2 8 2) peaks of SiO₂ phase were relatively large compared to the peaks of CaO and SO₃ phases while the Al₂O₃ and P₂O₅ are not detected. The monoclinic lattice parameters a = 0.8469 nm, b = 2.7336 nm, c = 0.6416 nm, and β = 89.207° were determined from the XRD patterns of the SiO₂ phase which are

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less than the reference. The powder samples have crystallite size and lattice strain 88.38 ± 38.08 nm and 0.15%, respectively. These preliminary studies can be used as an important platform for further research.

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