Structural Analysis of Bioceramic Materials for Denture Application

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Structural Analysis of Bioceramic Materials for Denture Application

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Abstract. Structural analysis has been performed on bioceramic materials for denture application by using X-ray diffraction (XRD), X-ray fluorescence (XRF), and Scanning Electron Microscopy (SEM). XRF is using for analysis chemical composition of raw materials. XRF shows the ratio 1 : 1 : 1 : 1 between feldspar, quartz, kaolin and eggshell, respectively, resulting composition CaO content of 56.78 %, which is similar with natural tooth. Sample preparation was carried out on temperature of 800 ^{o}C, 900 ^{o}C and 1000 ^{o}C. X-ray diffraction result showed that the structure is crystalline with trigonal crystal system for SiO_2 (a = b = 4.9134 Å, c = 5.4051 Å) and CaH_2O_2 (a = b = 3.5925 Å, c = 4.9082 Å). Based on the Scherrer's equation showed the crystallite size of the highest peak (SiO2) increase with increasing the temperature preparation. The highest hardness value (87 kg/mm^2) and match with the standards of dentin hardness. The surface structure was observed by using SEM also discussed.

Keywords: denture, chemical composition, crystal structure
PACS: 81.05-t

INTRODUCTION

Health sector is needed ceramic material that can be used for repair, reconstruction and replacement body parts, like bone or dental. Today, ceramics have been widely used to improve the quality of life of the people [1]. The utilization of ceramic materials, especially for denture application must be accompanied by an increase in the quality of the material. The quality of the ceramic material affected to the properties of dental ceramic such as; good color stability, biocompatible, ability to mimic the appearance of natural teeth, good wear resistance, and easy to treat. All these properties of dental material depend on the composition and structure of the constituent material. The microstructureal differences between the ceramic materials resulted in different structure, strength and even a slow crack growth [2].

Ceramic has the structure of inorganic and amorphous structures such as glass, or ceramic with crystalline structure. Microstructures of poly crystalline ceramics are always complex and are distinguished by the presence of grain boundaries (grain boundaries), microscopic (pores), imperfections, and multi-phase conditions.

To determine the composition of the ceramic base material in order to accordance with natural teeth, it is necessary to identify the composition of the bio-ceramic material and natural tooth be using X-ray fluorescence (XRF).

To determine the size of the crystals can be used Scherrer equation [3]:

$$B = \frac{K\lambda}{L\cos\theta} \qquad (1)$$

Where B = FWHM (Full Width at Half Maximum)
λ = wavelength radiation
K = 0.9
θ = Bragg angle
L = crystalline size

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METHODOLOGY

The materials are used for prepare a denture in this study is feldspar, quartz, kaolin and eggshell. All the material has a grain size of 0.05mm (300 meshes). The natural teeth are used as a reference in determining the composition. The X-Ray Fluorescence (XRF) is used to identification its chemical composition.

Sample preparation was done on temperature 800 ° C, 900 ° C, and 1000 ° C. The X-Ray Diffraction (XRD) is used to determine its crystal structure. The surface structure was observed by using Scanning Electron Microscopy (SEM). Hardness test was also performed on samples.

TABLE 1. The composition of raw material.

Sample	Mass (gram)			
	Feldspar	Quartz	Kaolin	Eggshell
G1	1.5	1.5	1.5	1.5
G2	1	2	2	1
G3	0.75	2.25	2.25	0.75
G4	0.857	2.57	1.716	0.857
G5	0.667	2.666	2	0.667

RESULT AND DISCUSION

The results of the identification the chemical composition using XRF can be seen in the following table.

TABLE 2. The results of X-Ray Fluorescence

Sample	Concentration of oxide (%)				
	CaO	Al_2O_3	Fe_2O_3	SiO2	K_2O
G1	56.87	3.04	-	39.50	-
G2	25.44	11.37	0.484	61.75	0.521
G3	18.54	13.47	0.521	66.61	0.508
G4	23.06	8.98	0.423	66.63	0.513
G5	15.64	12.80	0.432	70.32	0.480
Teeth	61.60	-	-	-	-

The sample G1 has concentration CaO close to natural teeth, which is 61.60 %. The sample G1 is a chosen sample for further analysis. Sample preparation was on temperature 800 °C, 900 °C, and 1000 °C.

The XRD show a crystalline structure. The Match program is used to determine its crystalline structure. The result is showed on figure 1 and table 3.

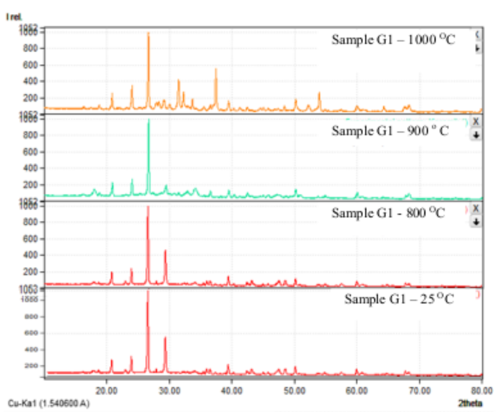
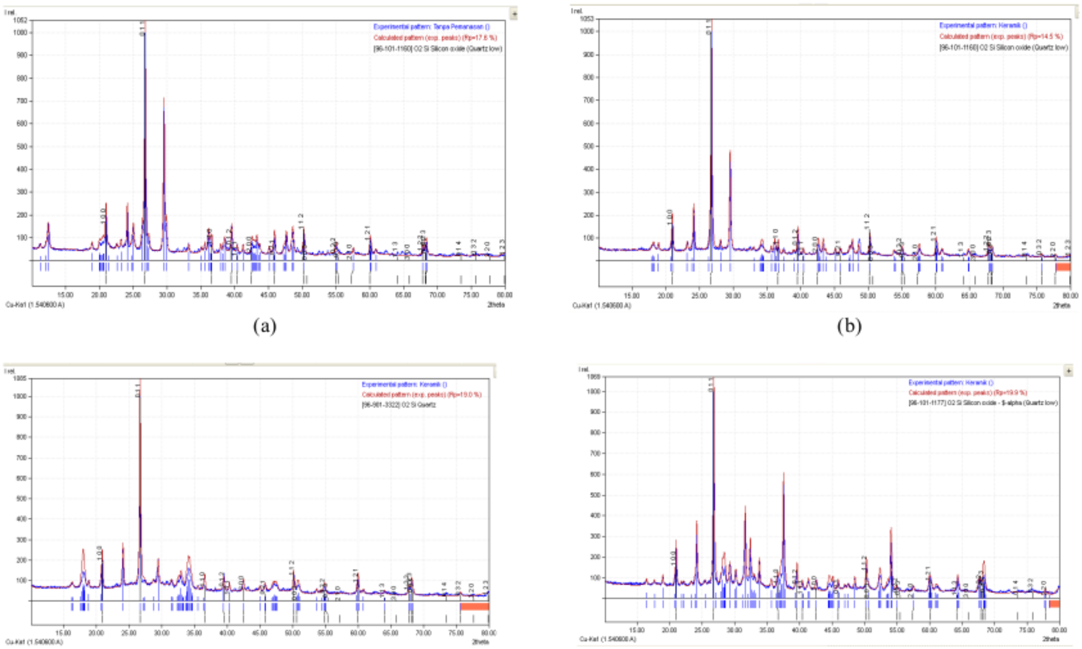


Figure 1. The XRD of sample G1

TABLE 3. The crystalline structure of sample G1

Temp. (°C)	Chemical component	Percentage (%)	Crystalline system
25	SiO_2	38.9	Trigonal
	$CCa0_{.936}$ $Mg0_{.064}$ O_3	32.5	Trigonal
800	SiO_2	63.2	Trigonal
	$CCaO_3$	36.8	Trigonal
900	SiO_2	87.7	Trigonal
	CaH_2O_2	12.3	Trigonal
1000	SiO_2	42.7	Trigonal
	$C_4Cl_2FN_2O_2S_5$	27.1	Monoclinic
	CaO	19.5	Cubic
	$Ga_6O_{25}Sc_4Sr_{10}$	10.7	Tetragonal

The percentage of SiO_2 is higher than other one. SiO_2 has trigonal structure. At 900 ° C the trigonal crystal system for SiO_2 (a = b = 4.9134 Å, c = 5.4051 Å) and CaH_2O_2 (a = b = 3.5925 Å, c = 4.9082 Å). The index Miller (hkl) of SiO_2 for different temperature preparation is showed on figure 2.



(a) (b) (c) (d)

Figure 2. The XRD sample G1 at temperature 25 °C, 800 °C, 900 °C and 1000 °C

The XRD data used the Full Width at Half Maximum (FWHM) of the most 3 highest peaks of XRD to calculate crystallite size on different temperature preparation. By using equation (1), it can be calculated crystallite size of the sample G1.

TABLE 4. The 3 highest peaks XRD at different temperature

Temperature (°C)	2 theta (deg)	d (A)	FWHM (deg)	Crystallite size (A)
25	26.7318	3.33220	0.18430	7.32
	29.5391	3.02159	0.17630	7.78
	24.1129	3.68785	0.14850	9.56
800	26.5668	3.35252	0.18690	7.62
	29.3563	3.03999	0.20350	7.04
	23.9424	3.71372	0.17460	8.16
900	26.6702	3.33975	0.17750	8.03
	24.0387	3.69906	0.17960	7.89
	20.8907	4.24882	0.19570	7.20
1000	26.6465	3.34267	0.17160	8.30
	37.4086	2.40205	0.17260	8.48
	31.4658	2.84083	0.25020	5.76

The calculations show that the crystallite size of the highest peak (SiO2) have increased along with the increase in temperature. The crystallite size 7.32 Å, 7.62 Å, 8.03 Å, and 8.30 Å, respective with room temperature, 800° C, 900° C and 1000° C. This proves that the temperature can affect the crystal structure of ceramic materials. Hardness test was also performed on samples G1 which the results can be seen in the following table.

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TABLE 5. The hardness test on sample G1

No.	Temperature (^{O}C)	Hardness (kg/mm^2)
1	800	16
2	900	87
3	1000	48

The test results showed that the samples G1 temperature 900 ^{o}C met the standard hardness of dentin (0.13 – 0.51 GPa) [4] Sample preparation on 900 ^{O}C gives the best result, and higher than standard. This result is in accordance with the data in table 3 shows that the highest percentage of SiO_2 is present in the sample at a temperature 900 ^{o}C, namely 87.7 %. The concentration SiO_2 is influence the hardness of ceramics. The G1 sample with temperature preparation 800 ° C and 1000 ° C have hardness 16 kg / mm^2 and 48 kg / mm^2, still in order.
Scanning electron microscopy (SEM) image is used on morphology of sample surface. It seems a nanostructure in a long range.

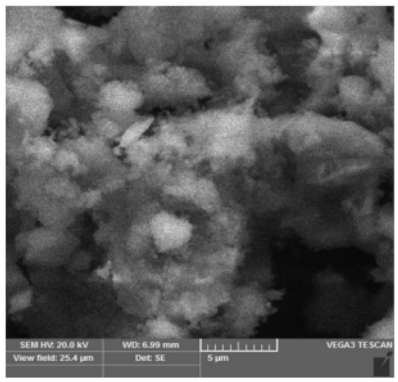

Figure 3. Scanning electron microscopy (SEM) image of surface sample

CONCLUSION

The composition of the ceramic material that is closest to the natural tooth composition is composition with a ratio of 1: 1: 1: 1 (feldspar : quartz : kaolin : eggshell) with CaO content reached 56.87%. X-ray diffraction result showed that the structure is crystalline with trigonal crystal system for SiO_2 (a = b = 4.9134 Å, c = 5.4051 Å) and CaH_2O_2 (a = b = 3.5925 Å, c = 4.9082 Å). Based on the Scherrer's equation showed the crystallite size of the highest peak (SiO2) increase with increasing the temperature preparation. The highest hardness value (87 kg/mm2) and match with the standards of dentin hardness.

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