

## Characterization of Central Kalimantan's Amethysts by Using X-Ray Diffraction

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**Abstract.** X-Ray Diffraction (XRD) is one of spectroscopy method that utilize X-Ray as an energy source in the phases identification. This method is used to characterize the type of amethyst of Sukamara, Central Kalimantan. In this paper, the crystallography of three types of Sukamara amethyst is reported. Samples was collected directly from the amethyst mine in the Ajang village in the District of Permata Kecubung. The samples consists of three types i.e. purple amethyst, black amethyst, and violet amethyst. The results show that quartz or silica ( $\text{SiO}_2$ ) is the main phase of the gemstone amethyst. Amethyst cell parameters are  $a = b \neq c$  and  $\alpha = \beta \neq \gamma$ , the crystal system is hexagonal. Amethyst average density is  $2.65 \text{ g/cm}^3$  and  $112.84 \text{ pm}^3$  cell volume. Peak FWHM value indicates that the degree of crystallinity of the black one is greater than that of the gasoline, while the degree of crystallinity of violet amethyst higher than purple amethyst.

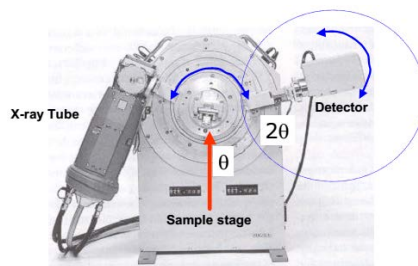
### 1. Introduction

Amethyst is a gemstone that has a main phase of  $\text{SiO}_2$ . Its refractive index is between 1544 - 1553, with hardness about 7 mosh. They are available in four main purple colors i.e. lilac, mauve, black and white. This gemstone is often given a symbol of sincerity, a sense of comfort and peace [1]. Although amethyst is well known gemstone and has been used for centuries, but the scientific identification of amethyst is still not reported. Therefore, for maintaining the commercial value of natural gemstones, it is necessary to identify the gemstone. By identifying gemstones we can differ a hardness level of various amethyst. This requires the analytical instruments to measure a hardness level. The instruments are often used in identifying gemstones are refractometer, polariscope, microscopy, and mini spectroscopy. In addition, there are advanced equipment also used for the identification of gemstones such as infrared spectroscopy, ultraviolet, and X-ray fluorescence (XRF) [2-4]. This paper shows scientific report of microstructural properties of amethyst gemstones. In particular, an X-Ray Diffraction (XRD) analysis was applied to determine the crystallographic characteristics of three types of amethyst, i.e. purple, violet and coffee amethyst. XRD method have been applied to scientist to characterized material worldwide such as for microstructural evolution and phase change of ceramics during processing [5-7]. Furthermore, this paper also reveals experimental and analytical methods to examine a hardness level of various amethyst based on XRD measurement results. Another method to determine material's hardness is by using Vicker's Hardness testing as reported previously to alumina ceramics [8-9]. Gemstones' hardness is one of their important property in addition to their beautiful colors. By detail scientific identification of these gemstones, we may be not only can maintenance their valuable properties but also can improve them.



## 2. Material and Method

XRD was utilized to characterize the microstructure of amethysts. The study was conducted through the following steps. Firstly, the collection and retrieval of stones containing three types of amethysts in Ajang village, Sukamara. Secondly, cutting and polishing to obtain the desired amethyst. Thirdly, take small part of each gemstone to be ground into. Lastly, performing XRD testing and analysis for samples. The XRD was setup at voltage of 40 kV with 35 mA in current. Angle shots start from 15-90 deg, a step size of 0.02 deg, time / step 0.5 s, and a scan speed of 0.04 deg/s.



**FIGURE 1.** Main parts of X-Ray Diffraction (XRD)

## 3. Results and Discussion

XRD testing conducted on purple, black and violet amethysts to obtain the characteristic of these gemstones. XRD data analysis was performed automatically by using software X'Pert Highscore Plus at the Laboratory of Central Materials and Advanced Minerals in State University of Malang followed by manual calculation. The results are described in detail in following parts.

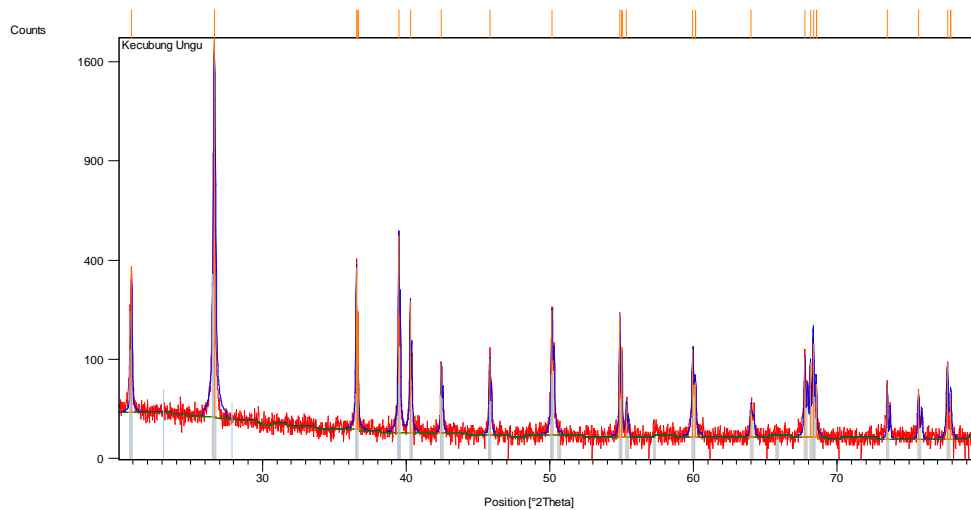
### 3.1 XRD analysis of purple amethyst

Purple amethyst stone is a gemstone which has a purple color and white fibers inside (Figure 2). This stone is often found in Kalimantan, Papua and West Java. For jewelry, this stone has been used since ancient Greece era [10].



**FIGURE 2.** Purple Amethyst

XRD result of purple amethyst can be seen in Figure 3. The pattern identified in purple amethyst is Quartz with a percentage of 100%, has the chemical formula  $\text{SiO}_2$ . Purple amethyst has a hexagonal crystal system with lattices parameters  $a = b = 4.9108 \text{ \AA}$  and  $c = 5.4028 \text{ \AA}$  where the angle between  $a$ ,  $b$  and  $c$  of  $\alpha = \beta = \gamma = 90^\circ$  and  $120^\circ$ . Volume amounted to 112.84 PM3 cell and density of  $2.65 \text{ g/cm}^3$ . There are 23 peaks detected in black amethyst, with the distance between atoms in cell units ( $d$ ) is  $1.22814\text{--}4.25524 \text{ \AA}$ . The total value of FWHM peak multiplied by the relative intensity is 26.0056, this value indicates the degree of crystallography. The size of the atomic crystal amethyst is between  $0.82 \times 10^{-9} \text{ m}$  and  $2.74 \times 10^{-9} \text{ m}$ .



**FIGURE 3.** XRD result of purple amethyst

### 3.2 XRD analysis of black amethyst

Black amethyst (Figure 4) is seen to be orange to reddish color if it is exposed by the light. It also has unique fibers therein. Black Amethyst is also often called as Wulung amethyst. In mineral quartz subject, black amethyst has similarities with Black Obsidian [11].



**FIGURE 4.** Black amethyst

Figure 5 shows XRD result of black amethyst. Crystallography parameter of black amethyst and purple amethyst are the same. The pattern identified in purple amethyst is Quartz with a percentage of 100%, has the chemical formula  $\text{SiO}_2$ . Coffee amethyst has a hexagonal crystal system with parameters of lattices  $a = b = 4.9108 \text{ \AA}$  and  $c = 5.4028 \text{ \AA}$  where the angle between  $a$ ,  $b$  and  $c$  of  $\alpha = \beta = \gamma = 90^\circ$  and  $120^\circ$ . Volume amounted to  $112.84 \text{ PM}^3$  cell and density of  $2.65 \text{ g / cm}^3$ . There are 24 peaks detected in black amethyst, with the distance between atoms in cell units ( $d$ ) is  $1.22817\text{-}4.24901 \text{ \AA}$ . The total value of FWHM peak multiplied by the relative intensity is 29.87297, this value indicates the degree of crystallography. The size of the atomic crystal amethyst is between  $4.2966 \times 10^{-11} \text{ m}$  -  $1.3886 \times 10^{-8} \text{ m}$ .

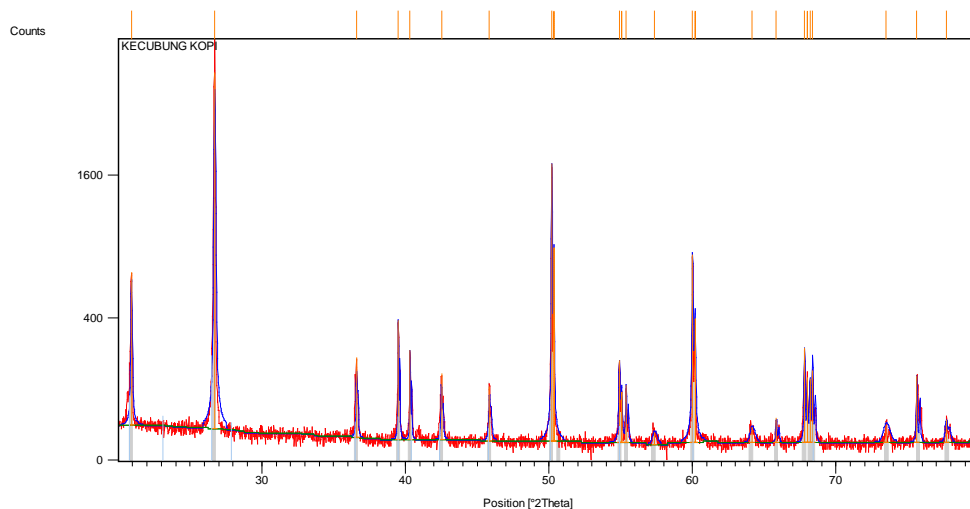


FIGURE 5. XRD result of black amethyst

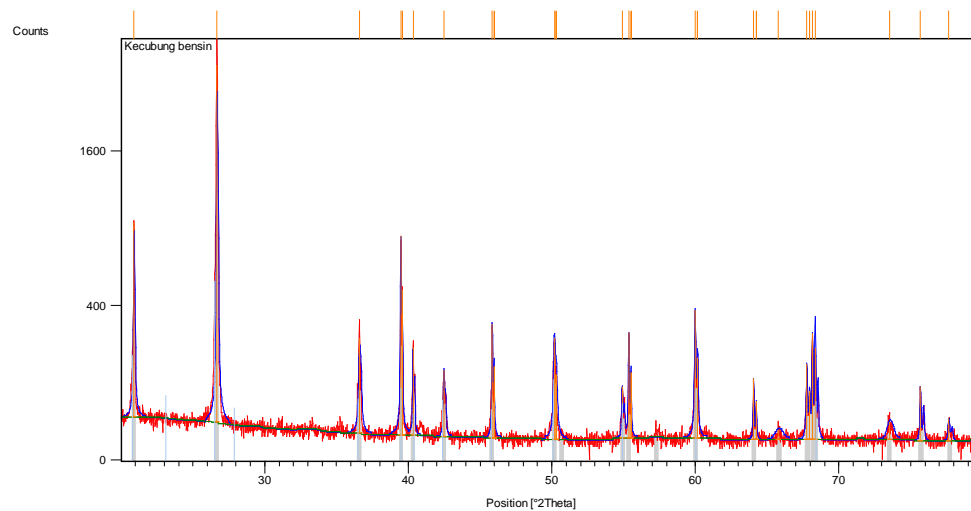
### 3.3 XRD analysis violet amethyst

One amethyst with a unique and very spectacular color is violet amethyst (Figure 6). This stone shines when exposed to the light and has ice-like fibers. However, when amethyst have crystallized, fibers do not appear.



FIGURE 6. Violet amethyst

Figure 7 depicts XRD result of violet amethyst. Crystallography parameter of black amethyst, violet amethyst and purple amethyst are the same. The pattern identified in purple amethyst is Quartz with a percentage of 100%, has the chemical formula  $\text{SiO}_2$ . Violet amethyst has a hexagonal crystal system with parameters of lattices  $a = b = 4.9108 \text{ \AA}$  and  $c = 5.4028 \text{ \AA}$  where the angle between  $a$ ,  $b$  and  $c$  of  $\alpha = \beta = \gamma = 90^\circ$  and  $120^\circ$ . Volume amounted to 112.84 PM3 cell and density of  $2.65 \text{ g / cm}^3$ . There are 26 peaks detected in violet amethyst, with the distance between atoms in cell units ( $d$ ) is  $1.22846\text{--}4.25143 \text{ \AA}$ . The total value of FWHM peak multiplied by the relative intensity is 28.28162, this value indicates the degree of crystallography. The size of the atomic crystal amethyst is between  $3.8808 \times 10^{-11} \text{ m} - 1.386 \times 10^{-8} \text{ m}$ . According to XRD analysis, three sample of amethysts has the same crystallographic characteristics, but vary in a number of peaks, the distance between the unit cells, the total value of FWHM and atomic crystals sizes. The greatest number of peaks is detected at violet amethyst followed by black and purple amethyst. The total value of FWHM peak of black amethyst multiplied by relative intensity greater than gasoline and purple amethyst. This value indicates hardness level of a gemstone [12]. Therefore, black amethyst has the highest hardness, followed by violet amethyst and purple amethyst. This conclusion is the consequence of their value of FWHM peak multiplied by the relative intensity of black amethyst, violet amethyst, and purple amethyst. The values are 29.87297, 28.28162, and 26.0056, respectively.



**FIGURE 7.** XRD result of violet amethyst

#### 4. Conclusion

From the analysis data from experimental results of XRD on coffee, gasoline, and purple amethysts, we can describe as follows:

1. Stone purple, coffee and petrol has a pattern of Quartz with a percentage of 100%.
2. The total value of FWHM peak of black amethyst multiplied by relative intensity greater than gasoline and purple amethyst, i.e. 29.87297, 28.28162, and 26.0056, respectively.
3. Black amethyst has the highest hardness, followed by violet amethyst and purple amethyst.

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