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Research Article

IDENTIFYING RELATED TO ANGLE 2θ WITH GRAIN SIZE OF CRYSTAL X RAY DIFFRACTION (XRD) ASSISTED SPREADSHEET EXCEL

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A B S T R A C T

This study aims to determine the relationship of theta angle to the grain size of the crystal x-ray diffraction with the calculation of the index field through the peaks of the spectrum produced. The data obtained in the form of intensity at various times and processed using spreadsheet excel to obtain the position of the diffraction peaks as well as an index field. Samples printed in pellet form and annealing at a temperature of 800°C. Characterization of the samples was done using XRD. XRD characterization results from the sample obtained and processed the data in graph form the relationship between the intensity of the 2 angel theta. XRD diffraction patterns are known to have some peaks and crystalline with a cubic structure, with a large particle size (Dv) and annealing at a temperature of 800° C for 1 hour which each amounted to 13.59 Å, 20.36 Å, and 52,99Å. It is known if the larger the particle size, the smaller the angle 2 theta and the greater the particle size, the average lattice strain (η) the greater the increase in line with annealing temperature.

INTRODUCTION

X-rays are a form of electromagnetic radiation having energies between 200 eV-1 MeV with a wavelength of between 0.5-2.5 Å. Wavelength almost equal to the distance between atoms in the crystal, causing the X-rays into a technique in mineral analysis. X-rays are formed when electrons are free to release some of the energy when interwoven interactions with other electrons orbiting the atomic nucleus or nuclei. The energy released from these electrons in the form of X-rays X-ray diffraction is a technique used to identify the presence of crystalline phases in materials and powders objects, and to analyze the properties of the structure (such as stress, grain size, phase composition crystal orientation and crystal defects) of each phase. This method uses an X-ray beam is diffracted as reflected from each field, respectively formed by the atoms of a crystal of the material. With a variety of angles arise, the diffraction pattern is formed representing the characteristics of the sample.

XRD (X-Ray Diffraction) is a tool to determine the characteristics of an index or a field contained crystal structure of various materials by utilizing X-ray scattering X-rays occurs when an electron beam of high kinetic energy free mashing metal which is a light source with permeabilities big. Then these electrons in the collision with the anode lead to emission of X-rays, so that the peaks appear, or visible from a material that is fired. With the peaks that are formed can be known from the field index of the materials used.

The structure of the material can be determined characteristics, either in the form of particles or solid, amorphous or crystalline, which is a core activity in materials science. The general approach is to examine the material carried by the beam of radiation or high-energy particles. In general, the nature of electromagnetic radiation, but also can be monochromatic or polychromatic. By utilizing the de Broglie hypothesis about the quality of the radiation frequency and momentum of a particle, then the idea of a wavelength can be applied in the excitation of electrons.

Symptoms of interference and diffraction is common in the field of light. Standard basic physics experiment to determine the lattice spacing is done by measuring the angle of the diffracted beam of light of known wavelength. Requirements to be met is a periodic grating and the wavelength of light has the same order as the lattice spacing to be determined. This experiment is directly attributable to the application of X-rays to determine the lattice spacing and the distance between atoms in the crystal lattice diffraction of crystal. The explaining is with three-dimensional lattice is quite complicated, but Bragg simplify it by showing that diffraction equivalent to a symmetrical reflection by the various crystal planes, provided that certain requirements are met. Utilization diffraction method plays an important role for the analysis of crystalline solids.

Crystals is the arrangement of atoms organized in three-dimensional space. The regularity of the arrangement occurs

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because the geometric conditions must be fulfilled, the provisions of the atomic bond, and the arrangement of the meeting. Although it is not easy to express how the atoms are arranged in a solid, but there are things that could be an important factor that determines the formation of the coordination polyhedra arrangement of atoms. This study aims to determine the relationship between 2θ with grain size (graiz size) of a material using XRD to determine the crystal structure.

METHODOLOGY

Methods of data analysis used in this research is to use excel spreadsheets, namely to create a chart when the laser beam on a material, it will show the intensity of the resulting graph. Then calculate the peaks of the spectrum using the following equation, to the corners of the diffraction peak on the crystal structure of the cube:

$$\frac{sin^2\theta_2}{sin^2\theta_1} = \frac{h2^2 + k2^2 + l2^2}{h1^2 + k2^2 + l1^2}$$

$$atau$$

$$\frac{sin^2\theta_1}{sin^2\theta_{min}}$$

Data obtained from such XRD X-ray diffraction intensity of the diffracted and angles 2θ. Each pattern appearing in an XRD pattern representing a crystal plane that has a specific orientation. Crystal size obtained is the average diameter of the heavy volume. The crystallite size can be calculated with the following Scherrer's equation:

$$Dv = \frac{K\gamma}{(b\cos\theta)}$$

RESULTS AND DISCUSSION

Below is a graph showing the data obtained 2θ relationship with intensity in a spreadsheet excel display as follows:

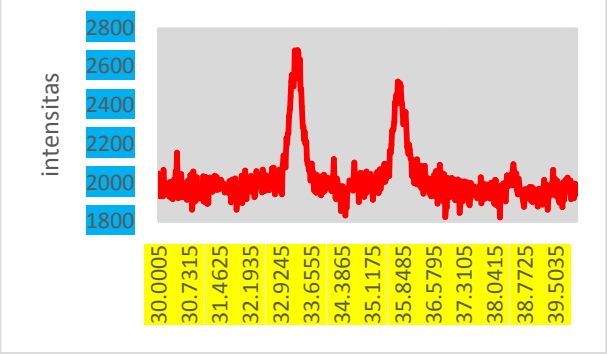

Figure 1 The graph display of the spreadsheet excel

Figure 1 shows the X-ray diffraction pattern after dianealing at a temperature of 800oC. Seen that after dianealing raised crests and can be calculated fields from peaks seen it. The tops indicates that the material is crystalline, which means having susuna irregular particles, although the peaks (hkl) which looks exactly the same. Thus the angle of each of the peaks that have been obtained in the form of 2θ can find the value of the distance between the field (dhkl) each peak for an unknown λ value of 1.544 Å. Berikuta dhkl value of each peak can be seen in the table below:

Table 1 Dhkl value of each peak

2θ angle (o)	Dhkl value (Å)
33.46	33.32
33.67	33.33
35.71	35.73
35.92	35.78

Table 1 above explains that the value of the distance between the field (dhkl) decreases with increasing magnitude of the angle theta. As for the average crystal grain size along with a large increase in 2θ can be seen in table 2 below:

Table 2 The value of the crystal grain size

2θ angle (o)	Crystal grain size
0.66	13:59
0:44	20:36
0:17	52.99

Table 2 above explains that the crystal size is inversely proportional to the angle 2θ, which saw the smaller the angle 2θ, the greater the grain size of the crest, where the relationship between the two can be seen from Figure 2 below:

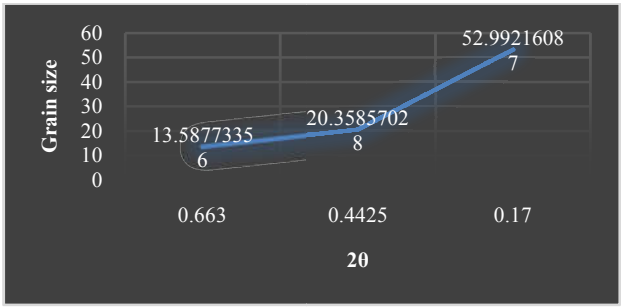

Figure 2 The relationship between the size of crystal grains 2θ

CONCLUSION

Distance field Crystals (dhkl) which has been found to decrease with greater angle theta. While the size of the crystal grain size of greater and greater as the angle theta. Besides the greater the particle size, the average lattice strain (η) greater and greater as the temperature rises.

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