Virtual X-Ray Diffractometer using Acoustic Wave for Material Science Education

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Abstract. In this research, virtual X-Ray Diffractometer (XRD) using acoustic wave for material science education has been proposed. Acoustic wave with frequency in ultrasonic range has been used to characterize acoustic crystal structures. The dimensions of model structure, which are in order of ultrasonic wavelength region, have been formed by three dimensional printer (3D printer) and cotton swab. The angle of ultrasonic source and detector have been swept to record reflected wave signal of each angle. The peak of each angle have been selected to calculate lattice spacing by Bragg's law and then compared with the implemented structure. The results show signal peaks of each diffracted angle. The experimental results showed that the lattice spacing values obtained from acoustic experiment were in good agreement with the measured values of the implemented structure. This virtual XRD system provide to be an efficient tool for understanding about crystal structure characterization.

1. Introduction

In present, material science research area is extremely popular and is applied directly to daily life. One powerful instrument which is important in material science research is X-Ray Diffractometer (XRD). The regime of XRD was firstly proposed by Lawrence Bragg and his father William Henry Bragg in 1913 [1]. XRD has been used in a number of material science research for characterizing the properties of materials [2, 3]. Since the cost of XRD is very expensive, the real concept of XRD is hardly explored with the instrument to determine crystallographic plane spacing in the class room.

In this paper, the concept of XRD has been demonstrated by using an experimental setup which we will describe in Section 3. In the experimental setup the ultrasonic acoustic wave has been used for characterizing structure formed by 3D printer and cotton swab. The magnified scale of this virtual system is a powerful tool to understand about material characterization in material science education.

2. Bragg's Laws

2.1. Bragg's law

Bragg's law is often used to explain X-Ray diffraction phenomenon and is defined as

$$2d\sin\theta = n\lambda\ . \tag{1}$$

Equation (1) relates diffracted angle (θ) to crystallographic plane spacing (d) and X-Ray diffraction wavelength (λ). As illustrated in figure 1, for the incident rays making an angle (θ) to the crystallographic set of planes, the reflected rays interfere constructively when the path difference ($2d\sin\theta$) is an integer multiple of X-Ray wavelength. With this technique, crystallographic planes within a crystalline material can be distinguished such that its crystal structure can be identified.

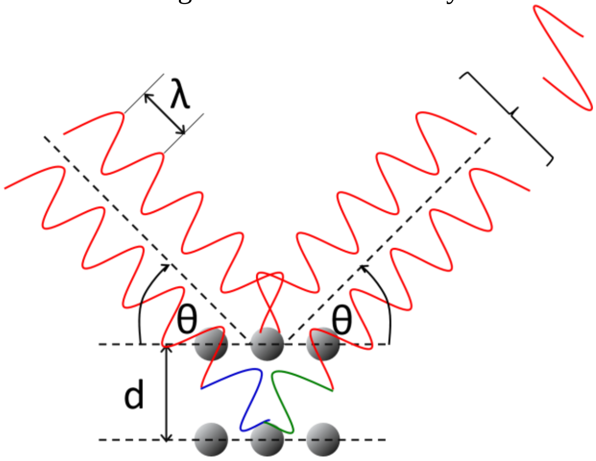


Figure 1. Diagram of Bragg's law.

2.2. Acoustic wavelength

Since this virtual XRD is used ultrasonic wave instead of X-Ray, acoustic wavelength (λ) have used to calculate in equation (1) can be obtained by [4]

$$\lambda = \frac{v}{f} \tag{2}$$

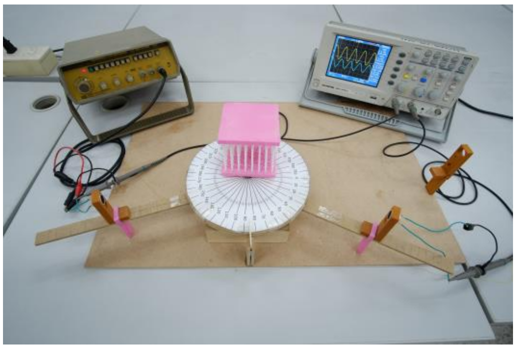
$$v = 331 + 0.6(t)\ , \tag{3}$$

where f is frequency of ultrasonic source and t is temperature of air in unit of Celsius degree (°C).

3. Experimental Setup

An experimental set-up and its diagram for this study, which consisted of function generator, oscilloscope, ultrasonic transmitter and receiver placed on the rotating arms, protractor ruler, and acoustic crystal as a sample structure, is shown in figures 2(a) and 3 respectively. The acoustic crystal is implemented by two-dimensional periodic arrangement of cotton swap sandwiched with two printed polymer plates (from 3D-printer) as illustrated in figure 2(b). Each unit cell of acoustic crystal is square shape and its lattice constant (d) is 9.6 mm. In experimental trial, the ultrasonic transmitter is driven by electric signal from function generator, then, an acoustic wave with ultrasonic frequency (41.93 kHz) would be emitted from the transmitter. Due to changing in temperature make an acoustic wavelength changed, the average room temperature during this experiment has been controlled to 25.0 °C. The initial wave obliquely incidents on the crystal plane at incident angle respecting to normal axis. Some parts of incident wave are reflected at each crystal planes at reflecting angle, which equals to incident angle in accordance to wave's reflecting principle, and detected by the ultrasonic receiver.

After that, the output electric signal of the receiver is generated and passed through to the oscilloscope for displaying reflected waves. In this study, the incident angles are varied from 10 to 80 degrees with 1 degree stepping-increment. The output voltages of ultrasonic receiver as a function of incident angle is plotted and curves fitted. According to the plot, finally, the output peak at any incident angle is paid attention. By using Bragg's law, the lattice spacing; *d* at any incident angle is calculated and compared with measured value.



(a)

(b)

Figure 2. (a) Experimental setup; (b) Model of crystal structure formed by 3D printer.

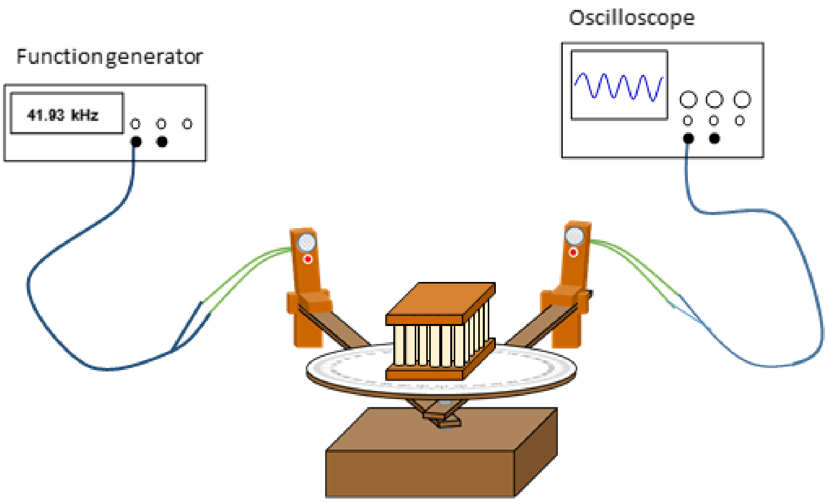


Figure 3. Diagram of experimental setup.

4. Results and Discussion

The results of reflected acoustic intensity of each swept angle from crystal structure has been shown in figure 4. There are two clear peaks intensity from reflected signal. One is at 25.5 degree and the other one is at 61 degree. These two peaks are the first and second order of reflected interference (n = 1 and n = 2 respectively). Reflected angle of the first peak (θ) at 25.5 degree and wavelength (λ) at 8.25 mm have been selected to determine crystallographic plane spacing (d) by using equation (1). This wavelength value is obtained by using equation (2) and (3) with t = 25.0 °C and f = 41.93 kHz. The crystallographic plane spacing determined by first peak is about 9.6 mm while crystallographic plane spacing from the imitate structure is 9.6 mm. In the same way, crystallographic plane spacing calculated with reflected angle of second order peak (θ) at 61 degree is about 9.4 mm. The error of first peak and second peak in this experiment when comparing with the real value of structure, which formed by 3D printer, are 0% and 2.08%, respectively. This discrepancy between real value and experiment value of lattice spacing might occur from the measuring process. Due to this virtual system using acoustic wave which cannot be observed by the eyes and hardly aligned it into a beam, the incident reflected angle might deviate from normal angle.

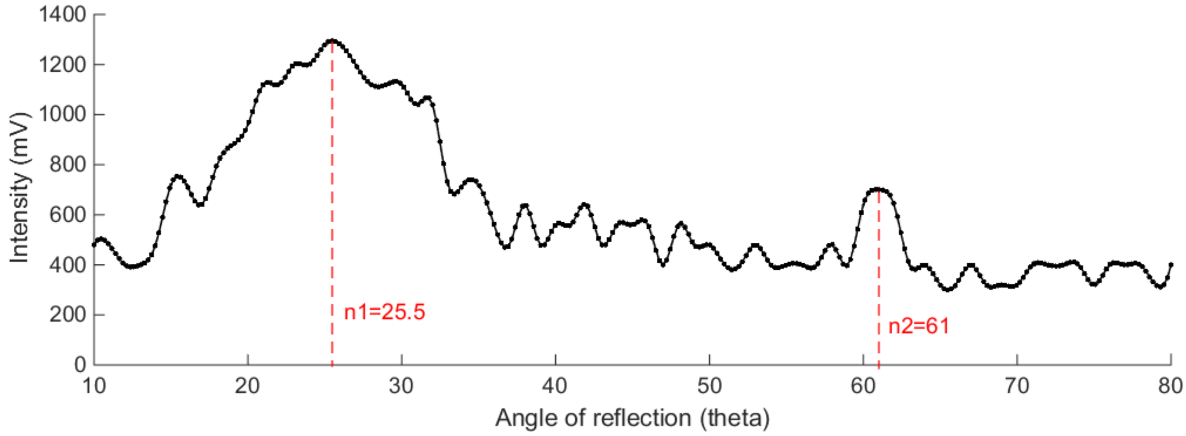


Figure 4. Experimental results of reflected wave signal at each angle; n1 is the first order of diffraction and n2 is second order of diffraction.

5. Conclusions

A demonstration of XRD concept using acoustic wave has been proposed in this innovation. Crystallographic plane spacing calculated by using both of two constructive peaks is in good agreement with the measurement value of implement structure. The magnified scale from angstrom to millimetre using acoustic wave instead of X-Ray range help the student clearly for understanding the concept of XRD, which is the important instrument in material characterization. Instructor or teacher could apply our system during teaching the concept of XRD by demonstrating in the laboratory. Magnified scale of this demonstrate system can help instructor to show how the wave incident on structure and then reflect with constructive interference at the angle that is in good agreement with Bragg's laws. Moreover, acoustics wave make safer while working in the experiment than using X-Ray. This virtual XRD system provide to be an efficient tool for understanding about crystal structure characterization.

References

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