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Simple Calculation based Method for Lattice Parameters in Tetragonal System using Powder X-Ray Diffraction Data

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Abstract: ***A crystal is a substance in which the particles are arranged in an orderly repeating, three dimensional system. The crystal lattice is the three dimensional arrangement of a solid crystal. There are seven crystal systems namely triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal and cubic. The seven crystal system consists of 32 classes. Among all tetragonal system seven point group or crystal class tetragonal pyramidal, tetragonal disphenoidal, tetragonal dipyramidal, tetragonal trapezohedral, ditetragonal pyramidal, tetragonal-scalenohedral, ditetragonal dipyramidal. Tetragonal system is characterized by different faces and bond angles. The edge length of crystal are represented by a, b and c. The angles at which faces intersect are represented by Greek letters α, β, and γ. For tetragonal systems like tin oxide (IV) are as shown in fig 1. They are designed are a=b≠c and α=β=γ. The dimensions are a=b=4.731Å and c=3.189Å along with α=β=γ=90^0. The present research paper gives the way of obtaining calculation for lattice parameter in tetragonal system like tin oxide (IV).***
Keywords: Crystal system, lattice parameters, tetragonal system, tin oxide (IV) etc.

I. . INTRODUCTION

Lattice constant determination is important tool to study crystal structure, phase identification, solubility range, physical properties and solvus curve determination [1]. A structure refers to internal arrangement of particle and not the external appearance of crystal lattice.

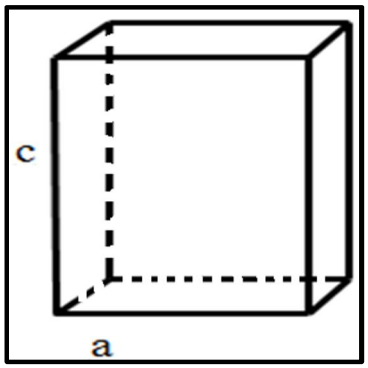

Fig. 1 lattice parameters representation in tetragonal unit cell system

Lattice parameters are the length between two points on the corners of a unit cell. There are some well-known method for determination of lattice parameters viz; Kossel method [2], the method of highly divergent method [3] and the bond method [4]. Quasi-multiple X-ray diffraction is one of the reliable techniques to determine lattice parameters. Some of the researchers developed and reported their significant contribution about Quasi-multiple X-ray diffraction in respective articles [5-8]. Quasi-multiple X-ray diffraction is based on measuring the angle between two diffraction peaks corresponding to two previously chosen reflections satisfying conditions similar to multiple X-ray diffraction in the coplanar geometry [8]. The extrapolation method in the derivation of accurate unit-cell dimensions of crystal lattice decorated by Nelson-Riley method has most versatile method to calculate lattice parameters [9]. Here in this article we are also able to calculate lattice parameters a & c in tetragonal system with simple interconverting method. The purpose of this article is to describe and develop a simple method of calculating lattice parameters from powder X-ray diffraction data on a crystal with known structure.

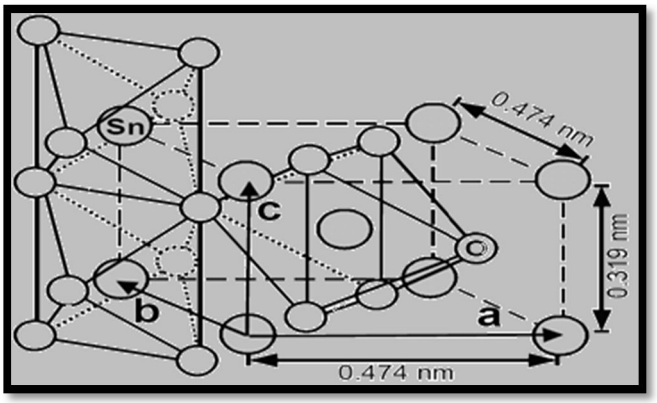

Fig 2. Crystal structure system of Tin oxide (IV)

II. MATERIAL AND METHODS

The method is simply to illustrate the significance of calculation of lattice parameters in tetragonal system like tin oxide crystal (SnO_2) and along with doped material along different planes with reference to JCPDS card No.41-1445. The standard values are a=b=4.731Å and c=3.189Å are obtained with standard data. The calculations are the part of interchanging the values and interconverting into one another as depicted in results and discussion.

III. RESULTS AND DISCUSSIONS

A. *Interconverting Method*

The calculations are as under,

According to standard value of lattice parameters given in J.C.P.D.S data

a=4.731Å and c=3.189Å, we have rearranged in mathematical expression,

$$\frac{a}{c} = \frac{4.731}{3.189}$$

On rearranging, $3.189 * a = 4.731 * c$

$$\therefore a = \frac{4.731}{3.189} * c$$

$$\therefore a = 1.483 * c \ldots\ldots (1)$$

Equation (1) can be written as

$$\therefore 1 * a = 1.483 * c$$

$$\therefore \frac{1}{1.483} * a = c$$

$$\therefore c = 0.674 * a \ldots\ldots (2)$$

B. *For Lattice Parameter, a=b in Tetragonal System*

For Lattice parameter, a=b

$$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

$$\therefore \frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{(0.674 * a)^2} \ldots from\ equation\ (2)$$

$$\therefore \frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{0.454 * a^2}$$

On cross multiplication to R.H.S

$$\therefore \frac{1}{d^2} = \frac{(0.454 * a^2)(h^2 + k^2) + l^2 a^2}{a^2(0.454 * a^2)}$$

$$\therefore \frac{1}{d^2} = \frac{(a^2)[\{(0.454)(h^2 + k^2)\} + l^2]}{(a^2)(0.454 * a^2)}$$

(a^2) Will get canceled on R.H.S

$$\therefore \frac{1}{d^2} = \frac{[\{(0.454)(h^2 + k^2)\} + l^2]}{(0.454 * a^2)}$$

$$\therefore d^2 = \frac{(0.454 * a^2)}{[\{(0.454)(h^2 + k^2)\} + l^2]}$$

$$\therefore d^2[\{(0.454)(h^2 + k^2)\} + l^2] = (0.454 * a^2)$$

$$\therefore \frac{d^2}{(0.454)} * [\{(0.454)(h^2 + k^2)\} + l^2] = (a^2)$$

$$\therefore (a^2) = \frac{d^2}{(0.454)} * [\{(0.454)(h^2 + k^2)\} + l^2]$$

Take square-root on both sides

$$\therefore (a) = \frac{d}{(0.674)} * \sqrt{[\{(0.454)(h^2 + k^2)\} + l^2]} \dots\dots (3)$$

C. For Lattice Parameter, c

Lattice parameter, c

$$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

$$\frac{1}{d^2} = \frac{h^2 + k^2}{(1.483c)^2} + \frac{l^2}{c^2} \dots\dots from\ equation\ (1)$$

$$\therefore \frac{1}{d^2} = \frac{h^2 + k^2}{2.199c^2} + \frac{l^2}{c^2}$$

$$\therefore \frac{1}{d^2} = \frac{c^2(h^2 + k^2) + 2.199(c^2 * l^2)}{2.199c^2 * c^2}$$

$$\therefore \frac{1}{d^2} = \frac{c^2[(h^2 + k^2) + 2.199(l^2)]}{c^2(2.199c^2)}$$

c^2 Will get cancel on R. H. S

$$\therefore \frac{1}{d^2} = \frac{[(h^2 + k^2) + 2.199(l^2)]}{(2.199c^2)}$$

$$\therefore d^2 = \frac{(2.199c^2)}{[(h^2 + k^2) + 2.199(l^2)]}$$

$$\therefore d = \frac{(1.483c)}{\sqrt{[(h^2 + k^2) + 2.199(l^2)]}}$$

$$\therefore d * \sqrt{[(h^2 + k^2) + 2.199(l^2)]} = (1.483c)$$

$$\therefore \frac{d * \sqrt{[(h^2 + k^2) + 2.199(l^2)]}}{1.483} = c$$

$$\therefore c = \frac{d * \sqrt{[(h^2 + k^2) + 2.199(l^2)]}}{1.483} \dots\dots (4)$$

Here above obtained equation (3) and equation (4) can be used to calculate the value of lattice parameters a and c in tetragonal system like tin oxide. The simplified formula shows that the magnitude of lattice parameters depend on nature of (h. k. l) planes and interplaner spacing (d).

IV. CONCLUSION

Here interplaner spacing is directly proportional to magnitude of lattice constant. More the value of d, more will be the value of lattice parameter a & c tetragonal system and vice-versa. We have successfully interconvert lattice parameters into one-another. The calculated values of lattice parameters in tetragonal system like tin oxide are concurrent with literature values and standard data. This method is useful and applicable for material scientist, ceramists, physicists, chemists and metallurgists.

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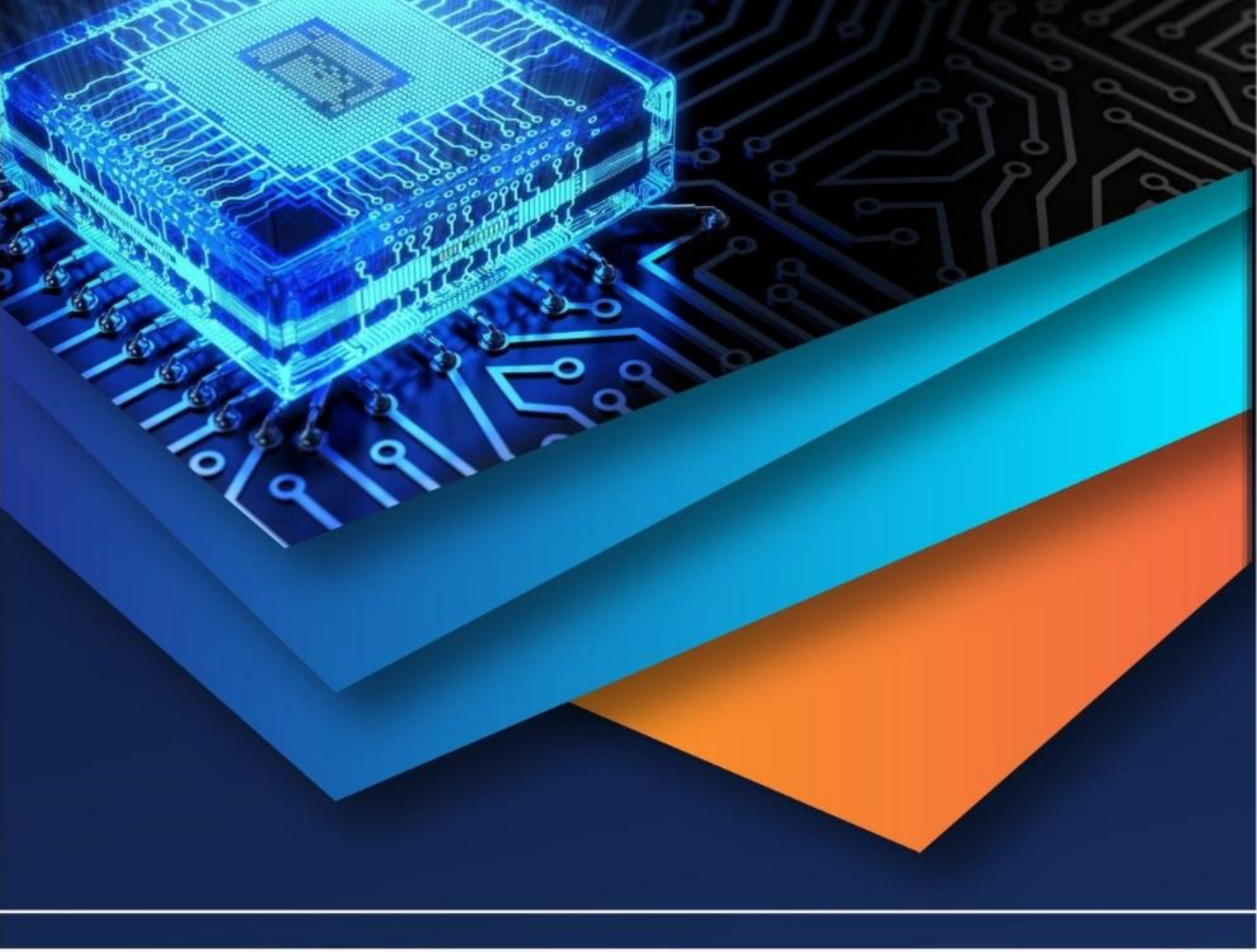

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