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Suggested Methodology of Molar Density along X-Ray Diffraction Spectrum for Nano-composite Mixture with Standard Formulae

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***Abstract:** One of the most important application of x-ray diffraction is to provide the structural details of the material to researchers. This technique is employed on massive scale to interpret the analysis of nano crystalline phases and to determine average crystallite sizes with the aid of diffraction angle or peak position and FWHM values on account of Scherer equation. The phenomenon of XRD can be explained as function of reflection of incident beam from the lattice planes. These results are also tuned for different molar density along XRD planes for any nanomaterial for molar mass and molar volume elaborated in this paper. We have tried to calculate molar density of composite mixture for nanostructured material in terms of molar mass and molar volume using XRD data of Intensity verses peak position and weight assigned for film material in composite form quantitatively.*
***Keywords:** Nano crystalline phases, XRD, peak position, molar density, molar mass, molar volume etc.*

I. INTRODUCTION

Material characterization includes different instrumental techniques such as XRD, scanning electron morphology, Fourier transform infra-red spectroscopy, ultra-violet spectrophotometer and Spectro-flurometry. Applications of nanomaterial are electrical [1], gas sensing [2], antimicrobial properties [3], photo catalyst [4], supercapasitors [5], transistors [6], humidity sensing [7] and much more. Different methods of material synthesis are also reported in different articles [8]. In XRD spectra intensity along plane either increases or decreases with peak position, one of the strong reason given to always atomic or molecular density along plane either increases or decreases along the peak. In this paper molar mass is evaluated for mixture using standard equations such as weight fractions in terms of number of moles and molar volume is obtained from PowderX software [9] by refining cell or by reitveld refinement [10] by X'pert highscore software [11].

II. MATERIALS AND METHODS

In this article a method was based on illustration to calculate atomic/molar density along XRD spectrum, for this purpose a screen printed tin oxide (SnO_2) composite for 1% zinc oxide (ZnO) material/sample was under consideration. Molar mass was calculated from mass of substance in grams to number of moles. The number of moles for molar mass was calculated from weights of material to molecular weight.

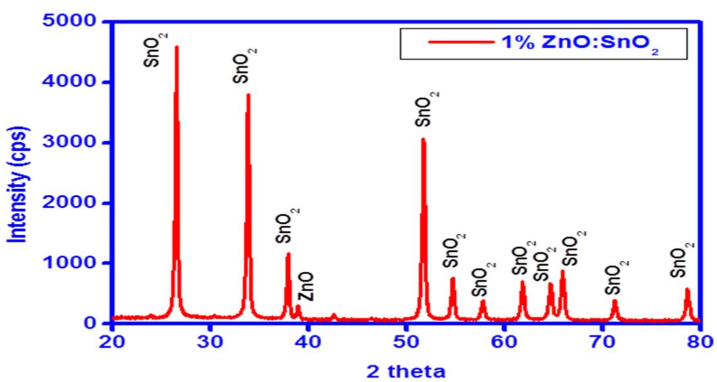

Fig 1. XRD pattern of 1% $ZnO:SnO_2$

Molar volume of 1% $ZnO:SnO_2$ composite material is obtained by considering above XRD pattern(fig 1.) Molar volume can be calculated or obtained from lattice parameters a, b and c. Molar volume is obtained from PowderX software by refining cell or by reitveld refinement by X'pert highscore software.

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III. RESULTS AND DISCUSSION

Density of material is the mass to volume ratio. When we consider molar density, it is defined as ratio of molar mass to molar volume. As every material prepared by any method in the form mixtures, composites, additives or doped into one another remain in their molecular state hence molar mass is considered. In mixture state, material remains as probably in compound and molar state not the atomic state (except by EDAX where we obtained values in atomic and weight percentage quantitatively and separately for each atoms of the material/composite material).

A. Molar mass/Molecular weight of Material can be Calculated from Following Equation

$$Molar\ Mass\ of\ \%\ ZnO{:}SnO_2 = \frac{Total\ Mass\ or\ weight\ of\ \%\ ZnO{:}SnO_2\ \ in\ grams}{Total\ Number\ of\ moles\ of\ \%ZnO{:}SnO_2}$$

……………………..(1)

B. Calculation for total number of moles of %ZnO:SnO$_2$

In 1% ZnO:SnO_2 composite mixture, 99% SnO_2 is present. Let the weight of 99% SnO_2 has 0.665 gm and 1% ZnO:SnO_2 has 0.00665 gm was mixed with tin oxide so as to form a mixture for screen printed film material.

To calculate total number of moles, we have the values of molecular weight of zinc oxide (ZnO) and molecular weight of tin oxide (SnO_2) i.e., 81.38 and 150.7088 respectively. The following formula is used [12].

$$Number\ of\ moles = \frac{Mass\ of\ substance}{Mass\ of\ one\ mole}$$

$$Number\ of\ moles\ of\ ZnO = \frac{Mass\ of\ ZnO\ in\ grams}{Molar\ Mass\ of\ ZnO}$$

$$Number\ of\ moles\ of\ ZnO = \frac{0.00665}{81.38}$$

$$Number\ of\ moles\ of\ ZnO = 0.000817154\ mol$$

Similarly

$$Number\ of\ moles\ of\ Tin\ oxide = \frac{Mass\ of\ tin\ oxide\ in\ grams}{Molar\ Mass\ of\ tin\ oxide}$$

$$Number\ of\ moles\ of\ Tin\ oxide = \frac{0.665}{150.7088}$$

$$Number\ of\ moles\ of\ ZnO = 0.004412\ mol$$

Total number of moles is the sum of Number of moles of zinc oxide (ZnO) and Number of moles of tin oxide (SnO_2)

$$Total\ Number\ of\ moles\ of\ ZnO{:}SnO2 = 0.004412\ \text{mol} + 0.000817154\ \text{mol} = 0.00522912\ \text{mol}$$

C. Calculation for Total Mass of Mixture

$$\text{Similarly}\ total\ mass\ of\ ZnO{:}SnO_2 = Mass\ of\ ZnO + Mass\ of\ SnO_2$$

$$Total\ mass\ of\ ZnO{:}SnO_2 = 0.00665 + 0.665 = 0.67164\ gm$$

By considering values obtained from part B and Part C, Equation 1, becomes,

$$Molar\ Mass\ of\ \%ZnO{:}SnO2 = \frac{Total\ Mass\ of\ \%\ ZnO{:}SnO2\ \ in\ grams}{Total\ Number\ of\ moles\ of\ \%ZnO{:}SnO2}$$

$$Molar\ Mass\ of\ \%ZnO{:}SnO2 = \frac{0.67164}{0.005229124}$$

$$Molar\ Mass\ of\ \%ZnO{:}SnO2 = 128.44\ gm$$

Molar mass of 1% ZnO:SnO_2 is 128.44 gms

D. To Evaluate the Molar Volume

Molar volume is the product of unit cell parameters a, b, and c along x,y and z axis in crystal lattice obtained from different software's like PowderX software by refining cell or by rut weld refinement or by X'pert highscore software in origin. After refining cell, lattice parameter were evaluated in following table

Table1. Refinement data for 1% $ZnO:SnO_2$

ZERO	LAMBDA	A	B	C	ALPHA	BETA	GAMMA
-0.026	1.54060	4.73661	4.73661	3.18588	90.000	90.000	90.000
0.002	0.00000	0.00018	0.00018	0.00012	0.002	0.002	0.002
VOLUME (A*B*C) : 71.47671 cc							

Molar volume obtained from refinement data shows value of 71.47671 CC. Cell volume was interpreted for the input of XRD data of 1% $ZnO:SnO_2$ into PowderX software after subtraction, subjected to baseline correction using different standard methods.

E. To evaluate molar density of 1% ZnO: SnO_2

As we know, from the definition of molar density [13],

$$Density\ of\ material = \frac{Molar\ Mass\ of\ material}{Molar\ Volume\ of\ material}$$

$$Molar\ \ density\ of\ 1\%\ ZnO:SnO_2 = \frac{Molar\ mass\ of\ 1\%\ ZnO:SnO_2}{Molar\ Volume\ of\ 1\%\ ZnO:SnO_2}$$

$$Molar\ \ density\ of\ 1\%\ ZnO:SnO_2 = \frac{128.44}{71.47671}$$

$$Molar\ \ density\ of\ 1\%\ ZnO:SnO_2 = 1.7975\ gm/cc$$

Thus Molar densities of any nanostructured material can be calculated with above method in terms of molar mass obtained from weights of composite material and molar volume obtained from reitveld refinement using different software**.**

IV. CONCLUSION

This paper will be our effort to suggest the basic reason behind high or low intensities observed in x-ray diffraction pattern along the planes. The main reason is total number of counts present along peaks. These counts are high for high intensities and low for low intensities. XRD pattern of different composite material may differ in intensities because of strain, dislocation densities, different interplaner spacing. The above values are obtained from different standard mathematical formulae for molar mass is 128.44 gm., molar volume 71.47671 cc and molar density 1.7975 gm/cc for 1% ZnO: SnO_2. The value of molar density for any composite material will be calculated from above standard equation and mathematical formulae. Molar density is directly proportional to molar mass and inversely proportional to molar volume. Molar density of any composite material in different percentage can be calculated with above formulaes.

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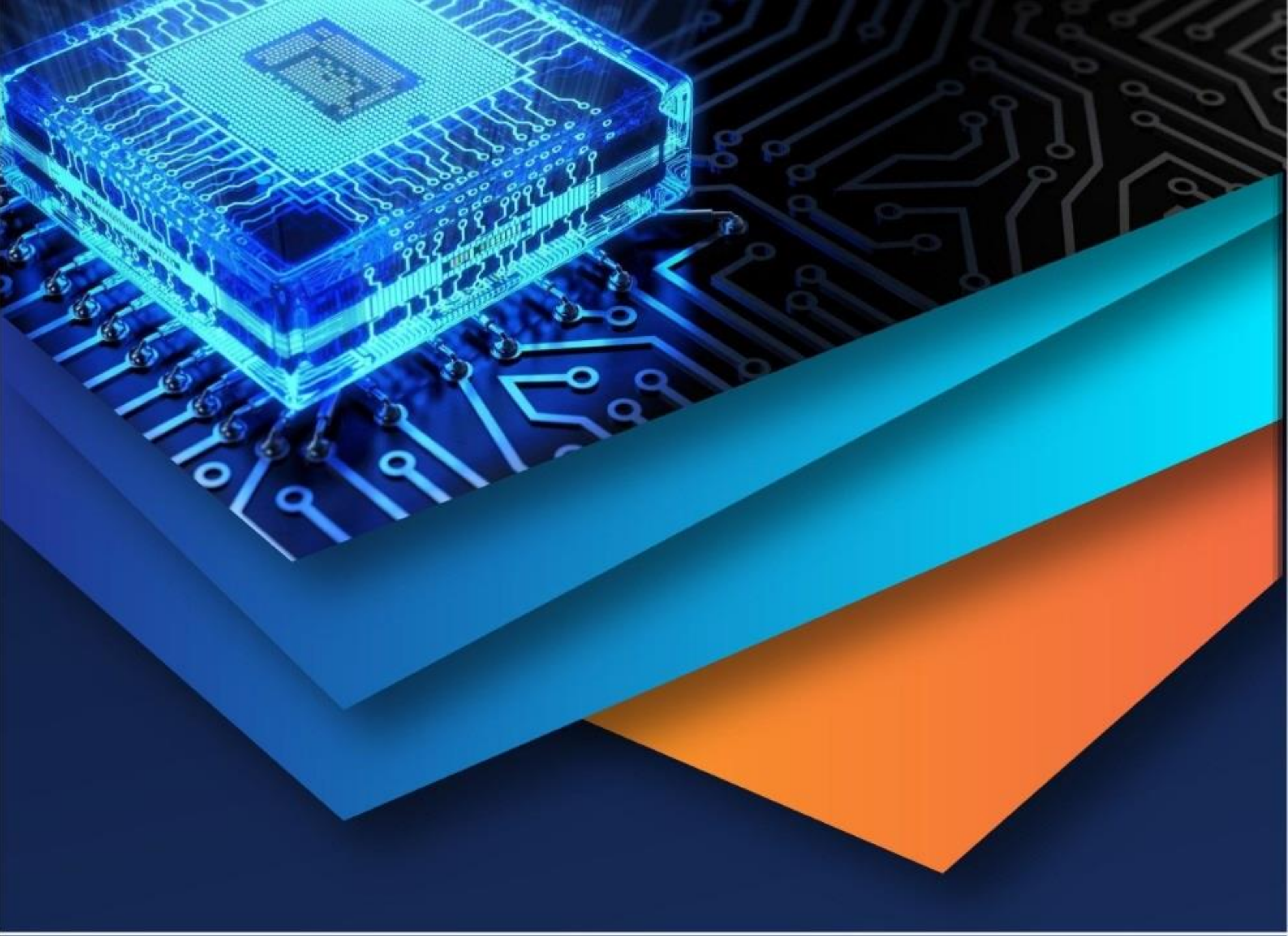

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