XRD, LPF and FTIR investigation of Mn-Bi alloy

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Abstract. High purity MnBi low temperature phase has been prepared and analyzed using X-ray diffraction, Lorentz-Polarization Factor and Fourier transforms infrared measurement. After synthesis of samples structural characterization has done on samples by X-ray diffraction, which shows that after making the bulk sample is in no single phase MnBi has been prepared by sintering Mn and Bi powder. The X-ray diffraction measurements were carried out using Bruker D8 Advance X-ray diffractometer. The X-rays were produced using a sealed tube and the wavelength of x-ray was 0.154nm (Cu K-alpha), and x-rays were detected using a fast counting detector based on Silicon strip technology (Bruker LynxEye detector). By Lorentz-Polarization Factor is affecting the relative intensity of diffraction lines on a powder form. The infrared absorption spectra of the alloys and intermetallic compound were measured at room temperature, in the wave number range 4000 to 400 cm \(^{-1}\) by a computerized spectrometer type Jasco FTIR-300 (JAPAN) using the KBr pellet technique. And by FTIR which shows absorption peaks of MnBi alloys.

1. Introduction
MnBi is a ferromagnetic inter-metallic compound with hexagonal crystal structure and the binary compound MnBi crystallizes into two phases, the lower temperature phase and the higher temperature phase. But at present the MnBi binary compound is in low temperature phase (LTP) [1]. The structural properties of these MnBi compounds have been studied by using X-ray diffraction, Lorentz-Polarization Factor and Fourier transforms infrared measurement of the low temperature phase (LTP) [2].

2. Experimental
One can start from highly pure fine powdered samples of Mn (Manganese) and Bi (Bismuth). Both of these were mixed in the calculated molar ratio of 45:55. These samples of different percentage of MnBi alloys were prepared by Solid state route method. The X-ray diffraction measurements were carried out using Bruker D8 Advance X-ray diffractometer. The X-rays were produced using a sealed tube and the wavelength of x-ray was 0.154nm (Cu K-alpha), and x-rays were detected using a fast counting detector based on Silicon strip technology (Bruker LynxEye detector). The diffraction pattern was scanned over the range 20 to 50 degree (2θ). The samples were characterized at room temperature using cuKα radiation. In this diffractometer, a radiation detector records the position and intensities of the various reflected line as a function of 20. Analysis of X-ray diffraction gives information about the different planes present in the specimen, lattice parameters and phase purity.

Lorentz factor is related to the volume of sample irradiated as a function of angle. The polarization factor accounts for increase scattering at low angles. For powder diffraction all the components of the Lorentz correction combine to give, when combined with the polarization correction, there is a pronounced enhancement of the low and high angle reflections relative to those at intermediate angles.
Lorentz-Polarization Factor is combination of two factors the Lorentz factor and the polarization factor that influence the intensity of the diffracted beam. And Lorentz-Polarization Factor is a Constant factor [4]. The Lorentz-polarization factor varies strongly with Bragg angle $\theta$, and the overall effect is that the intensity of reflections at intermediate Bragg angles is decreased compared to those at high or low angles. Now, Lorentz-Polarization factor is given by the relation-

$$\text{LPF} = \frac{(1+ \cos^2(2\theta))}{(\sin^2\theta \cos \theta)}$$

The infrared absorption spectra of the alloys and intermetallic compound were measured at room temperature, in the wave number range 4000 to 400 cm$^{-1}$ by a computerized spectrometer type Jasco FTIR-300 (JAPAN) using the KBr pellet technique. The samples were investigated as fine particles, which were mixed with KBr in the ratio (2:200mg powder to KBr respectively); the weighted mixture was then subjected to a pressure of 5t/cm$^2$ to produce clear homogeneous discs.

3. Results and discussion

3.1. X-ray diffraction studies:
XRD pattern of the available highly pure fine powder Mn and Bi and powdered samples such as MnBi in the atomic ratio 45:55, and shows the XRD pattern of MnBi compound before and after sintering (in figure 1). XRD peaks indicate the (hkl) values, and these values are showing the hexagonal crystal structure after indexed.

![XRD pattern of MnBi alloys](image)

(a) Sample-1  (b) Sample-2

**Figure1.** XRD pattern of MnBi alloys.

A close observation indicates that there is a systematic change in the FWHM of XRD peaks. The lattice parameter ($a=1.42\text{Å}$) and ($c=6.11\text{Å}$) of the MnBi alloys have been same before and after sintering. The particle size ($t$) of the MnBi intermetallic compound has been reported in Table1.

| MnBi alloy | Particle size | MnBi alloy | Particle size |
|------------|---------------|------------|---------------|
| Before Sintering | t(Å) | After sintering | t(Å) |
| Sample 1 | 301.84 | Sample 2 | 309.56 |

3.2. Lorentz-polarization factor studies:
The Lorentz-polarization factor is that which control X-ray intensity with respect to diffraction angle. Consider the X-ray intensity recorded on a piece of film as a crystal is rotated in an X-ray beam through the diffraction condition. The reflection is not infinitely narrow for a real crystal and the area under the curve is the integrated intensity. The integrated intensity is affected by the height and width of the curve [5]. These quantities are dependent on the Bragg angle as well as on the structure of the studied sample. When the Lorentz-polarization factor plotted with the $2\theta$ angle, the pattern is reported in Figure 2. In Figure 2 the LPF pattern of MnBi compound before and after sintering have been shown. In this pattern the LPF decreases as the $2\theta$ angle increases. In infrared spectroscopy, IR radiation is passed through a sample. Some of the infrared radiation is absorbed by the sample and
some of it is passed through or transmitted. The resulting spectrum represents the molecular absorption and transmission, creating a molecular fingerprint of the sample. Like a fingerprint no two unique molecular structures produce the same infrared spectrum.

![Figure 2](image.png)

**Figure 2.** Lorentz-polarization factor pattern of MnBi alloys.

### 3.3. Fourier transformation infrared spectroscopy studies:

The absorption peaks of MnBi alloys are in the Fourier Transform infrared Spectroscopy data. This is shown in figure 3 for both samples in which before sintering and after sintering.

![Figure 3](image.png)

**Figure 3.** Fourier transform IR spectra of MnBi alloys.

### 4. Conclusion

By the analysis of the X-ray diffraction pattern, one can conclude that both the samples are in crystalline form. Particle size is decreasing as one goes from before sintering to after sintering at the same temperature. Lorentz polarization factor decreases when the angle of diffraction increases. The absorption peaks of MnBi alloys are in the Fourier Transform Infrared Spectroscopy data. The fingerprints have no two unique molecular structures produces in the same infrared spectrum.

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### References

[1] Wohlfarth E P 1980 *Ferromagnetic Materials* (North-Holland).
[2] "Heusler alloy," *Encyclopedia Britannica Online*, retrieved Jan. 23, 2005.
[3] Yang J.B., Yelon W.B. and James W. J., Cai Q., Roy S. and Ali N. 2002 *J. Appl. Phys.* 91 10
[4] Suryanarayana C and Grant N M 1998 *X-Ray diffraction: a practical approach* (Springer).
[5] Reynold R C 1986 *Clays Clay Miner* 34 359.