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## Structural and Mössbauer spectroscopic effect of Titanium and Vanadium

Dr. R. K. Sharma M.S.J. Govt. College, Bharatpur-321 001, Rajasthan, India E-mail: <u>ravi.devansh@gmail.com</u>

**Abstract:** We report the effect of 3.3 atomic percent Titanium and Vanadium substitution for iron in iron diantimonide. X-ray powder diffraction patterns recorded at 300K suggest the presence of an orthorhombic structure similar to FeSb<sub>2</sub>. <sup>57</sup>Fe Mössbauer spectra measured at 300K suggest paramagnetic character. The variation in quadrupole splitting values compared to FeSb<sub>2</sub> for these two specimens indicate their nature being similar to the strongly correlated electron systems.

#### Introduction

FeSb<sub>2</sub> crystallizes into a C18 marcasite-type orthorhombic crystal structure, whereas TiSb, and  $VSb_2$  both possess a tetragonal structure [1, 2]. Recently, we have reported that Chromium can be substituted completely for iron [3]. In contrast, Mn can be substituted for iron upto 6.67 atom% in the  $FeSb_2$ retaining orthorhombic structure, and the magnetic properties of the  $Fe_{1-x}Mn_xSb_2$  alloy systems vary substantially [5] as predicted by Gonçalves da silva [6]. Petrovicet al. has reported very large  $\sim$  magnetoresistance for FeSb<sub>2</sub> in the temperature range  $40K < T_{cr} < 80K$  [7] and also a temperature-induced spin state transition within the Fe  $t_{2\alpha}$  multiplet based on The thermal expansion and heat capacity I measurements [8]. Since both Titanium (Ti) and Vanadium (V) possess nearly the same atomic radius as iron, one can expect from Hume-Rothery rules that one can precisely substitute Ti or V for Fe in FeSb<sub>2</sub>. Also, Ti and V are both 3d transition metals; one would like to observe the changes in the structural, electronic, and magnetic properties upon their substitution in pristine FeSb<sub>2</sub>. Therefore, we report the effect of 3.3 atom % Ti and V substitution in FeSb, using X-ray powder diffraction and Fe Mössbauer spectroscopic technique.

#### **Experimental details**

High purity ( $\approx 99.999\%$ ) elements were weighed in the stoichiometric proportion corresponding to  $Fe_{0.9}Ti_{0.1}Sb_2$  and  $Fe_{d.9}V_{0.1}Sb_2$  (compositions with 3.3 atom% substitutions of Ti and V for Fe) and sealed under vacuum ( $\approx 10^{-2}$  Torr) in quartz ampoules. The ampoules were kept in a Kanthal wire wound resistive furnace. Initially, the temperature was slowly raised from 300K to 1273K in the time interval of about 30 hours to ensure solid-state diffusion. Then, the temperature was fixed at 1273K for 30 hours to facilitate the complete mixing upon melting, and then subsequently, ampouleswere quenched into ice water. The furnace temperature was controlled by a temperature controller with an accuracy of about  $\pm 10$ K. The black ingot, thus, obtained was crushed into a fine powder and put again into an evacuated quartz ampouleand was annealed at 873K for 15 days and then quenched in water. The annealed ingot was crushed into a fine powder using an agate mortar and pestle.

X-ray powder diffraction patterns were recorded at 300K for the specimens using a Phillips 1840 model diffractometer (operated at 30 kV and 30 mA) by varying the 2 $\theta$  angle in the step of 0.02° from 10° to 90°.XRD data were analyzed using a standard program [9].

#### **Results and Discussions:**



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Fig 2:<sup>57</sup>Fe Mössbauer Spectra observed at 300 K for (a) Fe<sub>0.9</sub>Ti<sub>0.1</sub>Sb<sub>2</sub>(b) Fe<sub>0.9</sub>V<sub>0.1</sub>Sb<sub>2</sub> and (c) FeSb<sub>2</sub> Figure 1 shows the XRD powder patterns for Fe<sub>0.9</sub>Ti<sub>0.1</sub>Sb<sub>2</sub>Fe<sub>0.9</sub>V<sub>0.1</sub>Sb<sub>2</sub> and also for FeSb<sub>2</sub>. The powder patterns could be indexed using the "Powder X" indexing program [9], and the (hkl) indexing

corresponding to the experimentally observed peaks has been shown in it. For these specimens, the large intensity peaks corresponding to (011), (111), (211), (031), and (122) reflections in the increasing order of 20. This finding is similar to the one observed for FeSb<sub>2</sub>. Only three extra peaks could not be indexed corresponding to orthorhombic structure, and these are due to FeK<sub>β</sub> radiation. Since we did not observe any peaks corresponding to either Fe or Ti or V or Sb or any binary compound e.g. FeSb<sub>2</sub> or TiSb<sub>2</sub> or VSb<sub>2</sub>, the synthesized specimens Fe<sub>0.9</sub>Ti<sub>0.1</sub>Sb<sub>2</sub> and Fe<sub>0.9</sub>V<sub>0.1</sub>Sb<sub>2</sub>, therefore, possess an orthorhombic structure similar to FeSb<sub>3</sub> at 300K.

Fig.2 displays the <sup>57</sup>Fe Mössbauer spectra observed at 300K for  $Fe_{0.9}Ti_{0.1}Sb_2$ ,  $Fe_{0.9}V_{0.1}Sb_2$  and also for FeSb<sub>2</sub>. The experimental data points have been shown by dots, and the solid line is the computed envelope of the single quadrupole split doublet. The percentage absorption for  $Fe_{0.9}Ti_{0.1}Sb_2$  spectra is 4.1%, whereas  $Fe_{0.9}V_{0.1}Sb_2$  is about 4.6%. This may mean that the recoilless fraction and the Debye temperature should be distinctly different.

### Table 1:57Fe Mössbauer parameters at 300K,

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#### IS is given with respect to α-Fe

Sample	IS	QS	LW	χ <sup>2</sup>
Fe0.9Ti0.1Sb2	0.453(3)	1.259(6)	0.290(5)	2.628
Fe0.9V0.1Sb2	0.452(3)	1.260(6)	0.306(5)	2.566
FeSb <sub>2</sub>	0.452(3)	1.273(6)	0.294(5)	3.208

Table 1 gives the values of the Mössbauer parameters viz. Isomer shift (IS)

Table 1 gives the values of the Mössbauer parameters viz. Isomer shift (IS), quadrupole splitting (QS), line width (full width at half maximum, LW) and  $\chi^2$ , the goodness-of- fit parameter. The LW of the specimens' range between 0.290 - 0.306 mm/s which is comparable to the width 0.280 mm/s observed for the standard natural iron absorber. This justifies fitting the single quadrupole split doublet for the Mössbauer spectra for both Fe<sub>0.9</sub>Ti<sub>0.1</sub>Sb<sub>2</sub> and Fe<sub>0.9</sub>V<sub>0.1</sub>Sb<sub>2</sub>. This clearly indicates that at 300K, both these systems should be paramagnetic. The

Mössbauer IS does not change for these two specimens compared to

FeSb<sub>2</sub> suggesting that iron stays in the low spin state in these two specimens. There is considerable change in the quadrupole splittingfor these specimens compared to FeSb<sub>2</sub>. It may suggest that valence electron contribution to QS (resulting from the 3d electronic anisotropic distribution) has changed considerably. This may also suggest that the nature of the Fe<sub>0.9</sub>Ti<sub>0.1</sub>Sb<sub>2</sub>

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 $Fe_{0.9}V_{0.1}Sb_{2}$  systems should be similar to the and strongly correlated electron systems. We will measure these systems' magnetic properties to explore this behavior further.

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