



High performance FeTi – 3.1 mass % V alloy for on board hydrogen storage solution



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ABSTRACT

Single phase FeTi intermetallic and FeTi-3.1 mass % V alloy were synthesized by vacuum arc melting using high purity elemental constituents. The crystal structure of both, FeTi intermetallic and FeTi-3.1 mass % V alloy was found to be of CsCl-type. Under similar annealing conditions, crystallite size of FeTi-3.1 mass % V alloy was markedly smaller than that of FeTi intermetallic. Hydrogen absorption in FeTi intermetallic and FeTi-3.1 mass % V alloy was studied in a thermobalance attached to a Sieverts apparatus at a temperature of 327 K under 0.2 MPa hydrogen pressure. The hydrogen absorption in vanadium alloyed FeTi matrix was significantly faster than in the pure intermetallic. The maximum amount of hydrogen absorbed in the FeTi intermetallic and FeTi-3.1 mass % V alloy was of 1.2 and 1.1 mass % respectively.

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1. Introduction

In order to fulfill the increasing demands of a portable energy source and minimize the global warming effects associated with the use of fossil fuels, alternative energy options are being explored worldwide. The consumption of these fossil fuels based energy resources entails very high cost associated with degradation of environment due to green house effect. In this context, hydrogen based energy systems have advantages because of their high energy density, renewable and eco-friendly nature [1–5]. The availability of hydrogen at low cost in the form of water is the main driving force for the great amount of research work presently being carried out to achieve this energy transition. The issues associated with the development of hydrogen based energy system are neither the production nor the utilization of hydrogen but rather the storage system having: (a) safe and renewable high storage capacity, (b) light weight for easy transportation, (c) efficiently rechargeable and hydrogen release characteristics under moderate temperature and pressure conditions as well as (d) the cost factor to make them economically feasible for commercial applications.

Hydrogen storage in the solid form such as metal hydride or complex hydride is considered as the best option as compare to

liquid and gaseous storage methods on accounts of several reasons [6–12]. As a distinct class of materials, intermetallic compounds have been developed for the separation and storage applications. In this regard, FeTi is a prospective candidate among other AB₂ and AB₅ intermetallic systems for the use as a hydrogen storage medium. Although, maximum gravimetric hydrogen storage capacity of FeTi is mere 1.9 mass %, as shown in the Table 1, the output hydrogen pressure is superior to the widely investigated intermetallic compounds such as LaNi₅, ZrV₂ and Mg₂Ni. Moreover, their huge abundance and the low cost of constituent elements Fe and Ti are the compelling advantages for its commercial application. The main issue in the commercial application of FeTi intermetallic as hydrogen storage material is the sluggish kinetics of hydrogen absorption reaction at low working temperatures [13–19]. This issue may be resolved by making a FeTi composite or alloying it with a suitable element which may act as a suitable catalyst to enhance the kinetics of hydrogen absorption reaction even at low working temperatures. In this regard vanadium could be one of the effective alloying components because of its good catalytic properties [20]. The stronger interactive nature of vanadium towards hydrogen as compared to FeTi helps to increase the molecular dissociation of hydrogen leading to enhanced absorption kinetics [20–21]. Hydrogen absorption in FeTi is a diffusion controlled process [22–26] but the absorption is controlled by the surface reaction in the composites and alloys [27–32]. The reaction kinetics controlled by surface reaction is expected to be faster than that controlled by the diffusion process [33–40]. Similar changeover in the hydrogen

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Table 1
Comparison table of widely accepted intermetallic for hydrogen storage.

Type	Intermetallic	Hydrides	Wt. % H	P_{eq} (bar)	Temp (K)
AB ₅	LaNi ₅	LaNi ₅ H ₆	1.37	2	298
AB ₂	ZrV ₂	ZrV ₂ H _{5.5}	3.01	10 ⁻⁸	298
A ₂ B	Mg ₂ Ni	Mg ₂ NiH ₄	3.59	1	323
AB	FeTi	FeTiH ₂	1.89	5	303
BCC	TiV ₂	TiV ₂ H ₄	2.60	10	313

absorption mechanism of FeTi-3.1 mass % V alloy could be expected which may make it to enhance the absorption kinetics. In the present investigation, hydrogen absorption kinetics of FeTi-3.1 mass % V alloy has been studied and results are compared with FeTi intermetallic under identical conditions. In the following text, FeTi intermetallic has been designated as SA (sample A) and FeTi-3.1 mass % V alloy as SB (sample B).

2. Materials and methods

2.1. Materials

The specimens of sample A as well as the sample B were prepared by the vacuum arc melting technique using high purity iron granules (Euronorm make >99.99%), titanium sheet (Aldrich make >99.97%) and vanadium sheet (Aldrich make >99.98%). The constituents were thoroughly degreased before arc melting to minimize the possible contamination by metalloids. For preparation of FeTi intermetallic, components were taken in the required stoichiometric ratio and melted together with continuous stirring. The multiple arc melting was resorted to homogenize the charge. The homogeneity of the FeTi sample was analyzed by elemental mapping via micro-line scanning method using AIS-2100 CERON make SEM-EDS (scanning electron microscope–energy dispersive spectroscopy) techniques and result is shown in the Fig. 1. Four mass percentage of vanadium was added to FeTi and melted together in vacuum arc furnace which ultimately yielded to FeTi-3.1 mass % V alloy. The homogeneity and the elemental analysis of the samples were carried out by XRF (X-ray fluorescence) technique by exposing the different portion of the samples. In addition, the compositions of samples were also analyzed by wet-chemical method and the results are presented in Table 2. The analytical results obtained by all the techniques showed satisfactory

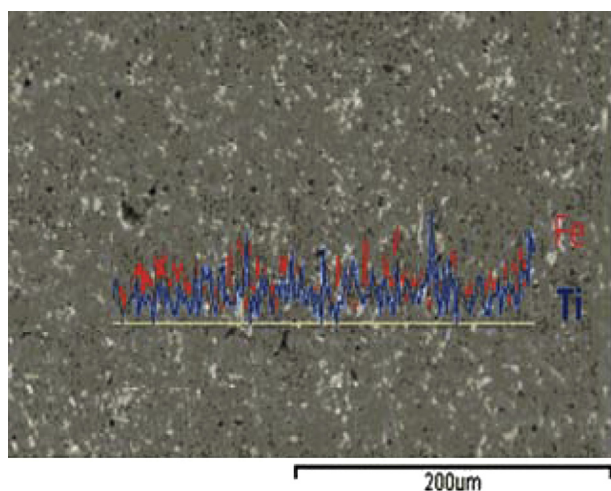


Fig. 1. SEM-EDS line scanning of the FeTi sample to check the elemental homogeneity. The analysis results revealed the Fe and Ti is uniformly mixed-up during arc melting and forms FeTi phase.

Table 2
Composition (mass %) of FeTi and FeTi-3.1 mass % V alloy analyzed by wet chemical and XRF analysis, oxygen and nitrogen were below 20 wppm.

Samples	Fe (mass %)	Ti (mass %)	V (mass %)
1 (FeTi)	55.14	44.85	–
2 (FeTi-3.1 mass% V)	53.23	43.17	3.10

agreement. The results indicates that Fe and Ti were approximately in the atomic ratio of 1:1 in sample A and 0.99:1 in sample B. The phase analysis of the samples were performed by Philips make PW 1830 diffractometer using Cu-K_α radiation (λ : 1.5418 Å). The XRD analysis of sample A indicates single phase FeTi intermetallic as presented in Fig 2a. Identical phase was observed for the sample B with an average XRD peaks shift of 0.8° with respect to FeTi as presented in Fig 2b. These samples were sliced into the specimen of dimension 4 × 4 × 0.2 mm³ with the help of EDM (electronic discharge cutting machine). All the specimens were cleaned and polished up to three delta finished surface using high grade emery paper followed by diamond paste. These polished specimens were used for all the hydrogen charging experiment and analysis purposes. For the microstructural examination under an optical microscope, the specimens were chemically etched by 1% chromic acid solution. The microstructures of both sample A and sample B are presented in Fig. 3a and b respectively.

2.2. Hydrogen charging

A modified thermobalance attached to a Sieverts apparatus was used for all the hydrogen charging experiments. A schematic diagram of the apparatus used in the present investigation is shown in the Fig. 4. The apparatus consists of a reaction chamber made-up of transparent quartz, high vacuum system, CI make modified thermobalance, sample hanger along with sample pan made of quartz and automated controlled furnace. Along with the furnace temperature, sample temperature was also measured separately by placing a K-type thermocouple near to the sample pan. The system has an EPC (electronic pressure controller) to control the hydrogen

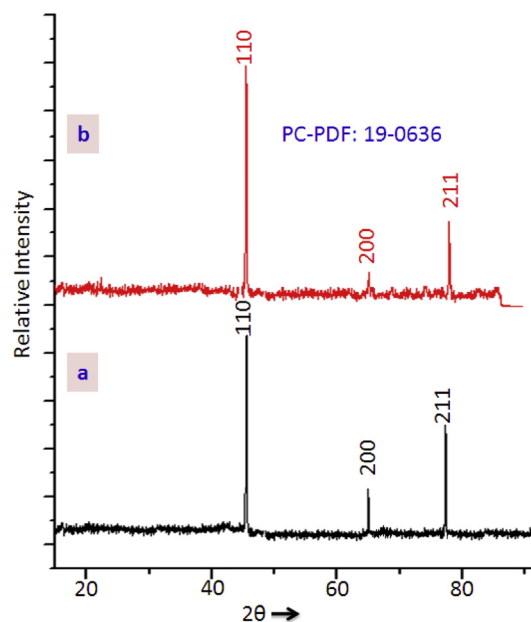


Fig. 2. XRD analysis of FeTi intermetallic and FeTi-3.1 mass % V alloy. An XRD peak shifts of about 0.8° was observed which indicates the solid solubility of vanadium in the FeTi intermetallic.

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