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Thermoelectric Performance of Fe_2VAl/CNT-Based Alloys

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Introduction

A promising material to produce thermoelectric power near the room temperature is Fe_2VAl Heusler alloy. In the Fe_2VAl system, the doping elements, for example the Si substitution for Al site in the n-type and Ti instead of V in p-type, can be used to simultaneously increase the power factor and control the type of conduction. Owing to their thermal conductivity that could reach ~ (28 W/mK), its efficiency of thermoelectric energy conversion is significantly smaller. Due to its superior mechanical properties, extreme mobility of the charge carrier, and small band gap energy, carbon nanotube (CNT) is one of the possible interesting TE materials. As known, the CNTs doping effect related to the characteristics of Heusler alloys was not yet studied. Considering the growing interest in studying the CNTs effects on the thermoelectrical properties of compounds [16], we present a systematic study on selected materials based on p-type Heusler alloys of Fe_2VAl system and added CNTs to the alloys. In the current study, we investigate the effect of CNT doping on the thermoelectric properties of $Fe_2V_{0.9}Ti_{0.1}Al$ alloys.

Materials and methods

Crystalline alloys of nominal chemical composition of p-type $Fe_2V_{0.9}Ti_{0.1}Al$ were synthesized from initial chemical elements of high purity (99.999%) by arc and induction melting in argon atmosphere. At a high temperature of 1073 K, the prepared samples were annealed for 72 hours in evacuated quartz tubes and crushed to a fine powder and divided into two components. Carbon nanotubes (CNTs) were added to the powder of the as prepared ingots in an amount of 2% by weight.

The CNTs were mixed to the powder of the prepared alloy in a ball mill with a 450-rpm rotation speed for 4 h. On a spark plasma sintering (SPS) unit Labox 650, Sinter Land, the powders were mixed under a vacuum at a pressure of 50 MPa, and temperatures of 1023 K. Circular disk-shaped synthetic samples were annealed for two days at 1073 K. The phase composition of the concerned samples was analyzed on a Difrey 401 diffractometer using CrKα (λ = 2.2909 A˚) radiation. For qualitative elemental analysis, a Tescan scanning electron microscope (SEM) with energy dispersive analysis was used. From the thermal diffusivity measured using the laser flash method on a Netzsch LFA 447 unit in the temperature range of 300–473 K, the thermal conductivity of the alloys was estimated. Utilizing the four-probe approach and differential techniques, respectively, the temperature dependences of electrical conductivity and thermoelectric EMF coefficient were evaluated within the temperature range of 300–473 K.

The surface structure of the obtained Samples are shown in Fig. 1.

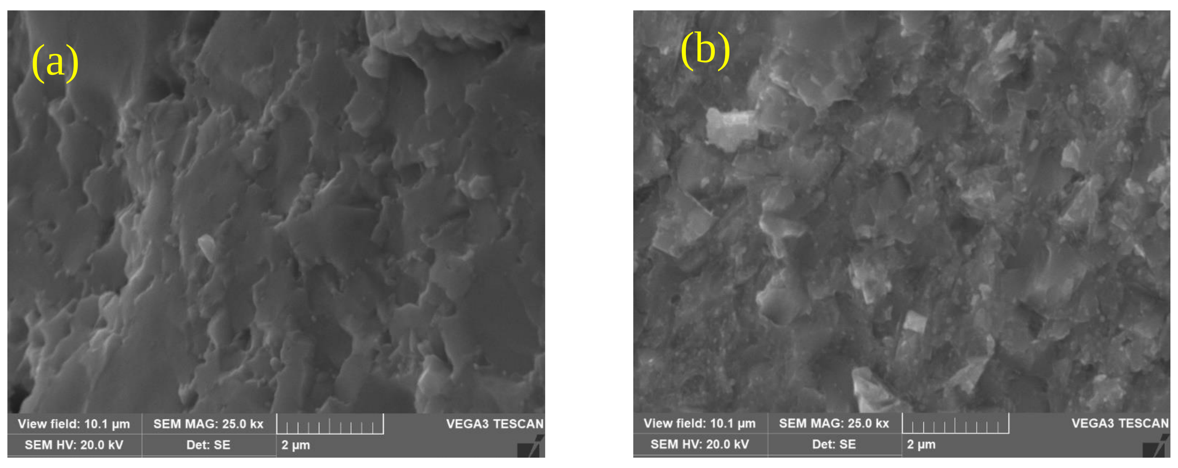

Fig. 1. SEM micro images of $Fe_2V_{0.9}Ti_{0.1}Al$ system (a), and $Fe_2V_{0.9}Ti_{0.1}Al$/CNT (b)

Results

The XRD measurements were performed on sintered $Fe_2V_{0.9}Ti_{0.1}Al$ (FVA) and $Fe_2V_{0.9}Ti_{0.1}Al$/CNT (FVA-CNT) alloys to examine the crystal structure and identify the different phases that comprise the obtained samples. As can be seen in Fig.2 (left), the Fe2VAl Heusler-type (L21) structure was recognized for all the diffraction peaks from each sample. XRD results for the FVA-CNT samples did not indicate any impurity phases. The positions of the main peaks correspond to the cubic structure with the lattice parameter a = 3.49093A˚ for FVA and a = 3.48816 A˚ for FVA-CNT, respectively. Quantitative analysis of composition constituents, in terms of the percentage of all elements present in each sample was conducted by the energy x-ray spectroscopy (EDX). The actual elemental percentage, with different atomic ratios, is in good agreement with the corresponding nominal levels, according to EDX data, Fig.2 (right)

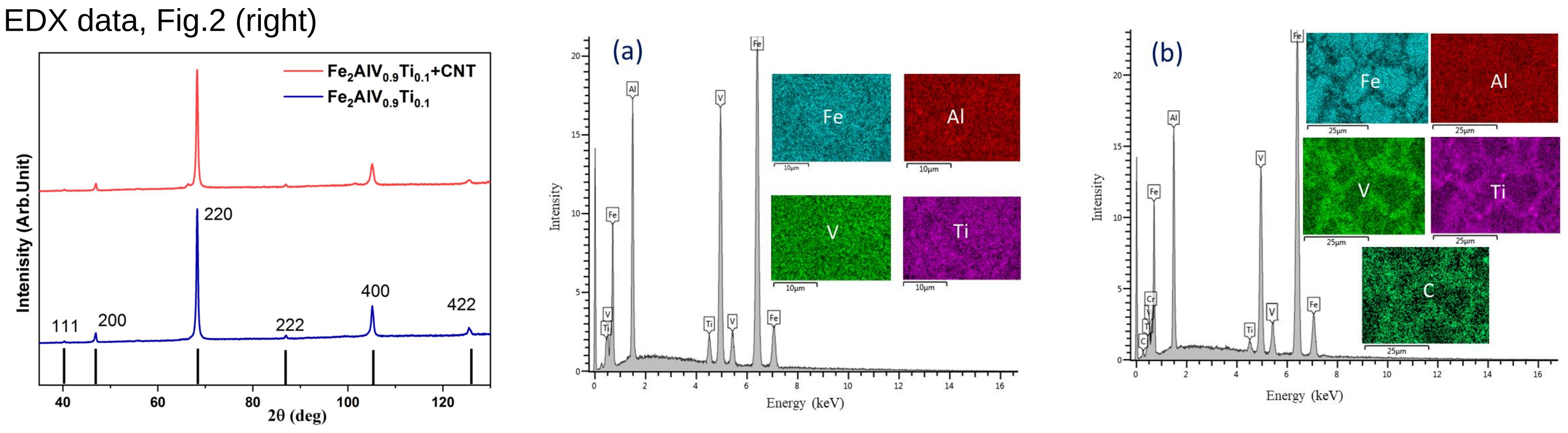

Fig. 2. The patterns of XRD diffracted from the sintered alloys (left), and EDAX spectra of (a) the $Fe_2V_{0.9}Ti_{0.1}Al$ and (b) the $Fe_2V_{0.9}Ti_{0.1}Al$/CNT

The thermoelectric parameters, Seebeck coefficient S, and the electrical conductivity σ within the range of temperature from 320 to 465 K for the samples $Fe_2V_{0.9}Ti_{0.1}Al$, and $Fe_2V_{0.9}Ti_{0.1}Al$/CNT are presented in **Fig. 3 (a, b)**. The achieved results show that the CNTs doping strongly affected the thermoelectric properties of Heusler alloys. **Fig. 3a** shows remarkable increase in the value of σ as the temperature increase for both samples. $Fe_2V_{0.9}Ti_{0.1}Al$/CNT samples showed higher σ than the alloy without CNTs. FVA-CNT had an electrical conductivity maximum of 3400 $\Omega^{-1}cm^{-1}$ at 465 K, while a value of 1950 $\Omega^{-1}cm^{-1}$ for the FVA sample**, Fig. 3a**. The enhancement in the electrical conductivity for FVA-CNT alloys strongly contributes to increased thermoelectric efficiency.

Fig. 3b shows the Seebeck coefficient variation of the two samples within the temperature range. As clearly seen, Seebeck coefficient decreases with increasing the measuring temperature. Adding CNTs to FVA system is accompanied by an enhancement in the values of S by almost one order of magnitude. Fe2V0.9Ti0.1Al/CNT had a maximum Seebeck coefficient of 70 μV K^{-1} at ~315 K, that is higher compared to the FVA sample.

The significant effects upon the adding of CNTs on the properties of the thermoelectric FVA Heusler alloys **(Fig. 3)** can be qualitatively explained considering the type of conductivity of the CNTs themselves. Considering that CNTs are p-type conductors with the Seebeck coefficient at room temperature ~ 20−40 μV K^{-1}, their addition to the Heusler alloy $Fe_2V_{0.9}Ti_{0.1}Al$ which is p-type, leads to a relatively high change in both S and σ **(Fig. 3)**.

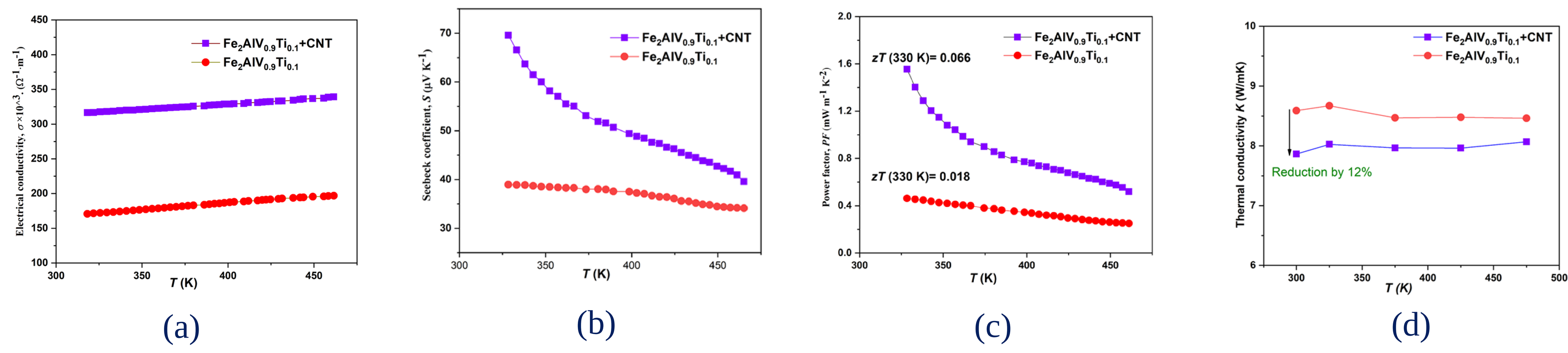

Fig. 3. From left to right, the electrical conductivity (a), Seebeck coefficient (b), the power factor (c), and thermal conductivity (d) vs. temperature for $Fe_2V_{0.9}Ti_{0.1}Al$ and $Fe_2V_{0.9}Ti_{0.1}Al$ /CNT samples

The power factor, PF = S2σ is another variable that fits the behavior of the Seebeck coefficient. It is evident that when temperatures rise, the power factor falls, as shown in **Fig.3c**. Additionally, within the investigated temperature range, the CNT doped samples exhibit an improvement in the power factor compared to the un-doped ones. With a value of 1.6 mW m^{-1} K^{-2} at 325 K, the $Fe_2V_{0.9}Ti_{0.1}Al$ /CNT alloy had the highest power factor. Although p-type Fe2V0.9Ti0.1Al /CNT sample have the largest power factor, however, has lower thermal conductivity compared with $Fe_2V_{0.9}Ti_{0.1}Al$ samples, **Fig.3d**. From results, the samples with CNT doping have the highest ZT. Consequently, the FVA-CNT sample at 320 K's figure of merit ZT increased by almost 250%, from 0.02 for FVA to 0.07. Due to the lower thermal conductivity and higher power factor, we were able to produce an alloy based on Fe2VAl/CNT that had higher ZT values than the pristine bulk alloy. Although we obtained a ZT value of 0.07 in the current study which is relatively small, we have the opportunity to improve it by the optimization of the CNT parameters.

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Conclusion

It was revealed that CNTs addition improved the electrical conductivity and thermoelectric power. $Fe_2V_{0.9}Ti_{0.1}Al$ /CNT showed a reduced thermal conductivity. The improvement in the figure of merit is caused by the decrease in thermal conductivity and the rise in power factor. At room temperature, the $Fe_2V_{0.9}Ti_{0.1}Al$ /CNT alloys' figure of merit *ZT* achieved 0.07. Following these results in the future, it looks interesting to study the efficiency of the thermoelectric materials with different carbon nanotubes content, which will make it possible to determine the percolation threshold and optimizing the thermoelectric properties of Heusler compounds with carbon nanotubes content. We anticipate that the great endurance of the Heusler alloy and the low cost of the CNT element will be advantageous in practical systems.