# Thermoelectric properties of $FeV_{0.955-x}Hf_{0.045}Ti_xSb$ half-Heusler phase

○Kévin Delime-Codrin[1], Tsunehiro Takeuchi[1,2]
[1] Toyota Technological Institute, Nagoya 468-8511, Japan
[2] IMaSS, Nagoya University, Nagoya 464-8603, Japan
**E-mail :** delime-codrinkevin@hotmail.fr

## Introduction

The FeVSb half-Heusler phase (HH-phase), consisting solely of cheap and non-toxic elements was studied as a new thermoelectric material. By using theoretical calculations(1), we found that the FeVSb HH-phase is capable of possessing a large figure of merit $ZT = S^2T/\rho\kappa$ exceeding 0.80 at a p-type condition at 700 K. To confirm this prediction, we prepared $FeV_{1-x}Ti_xSb$ HH-phases alloys and found that the figure of merit *ZT* of $FeV_{1-x}Ti_xSb$ HH-phases showed almost the same *ZT*-value as that predicted; $ZT = 0.63$ for $FeV_{0.80}Ti_{0.20}Sb$ at 700 K. Notably, this value is the highest ever reported(2) for FeVSb-based HH-phases.

The partial element substitutions, such as (Ti, Nb) for V and Co for Fe, were reported to be an efficient way to drastically reduce the lattice thermal conductivity of FeVSb-based HH-phases(2, 3). Otherwise, we realized that the influence of heavy element partial substitution such as Hf, Ta or W for V wasn't investigated yet. In this study, therefore, we fabricated HH-phases at the compositions of $FeV_{0.955-x}Hf_{0.045}Ti_xSb$ ($0 < x < 0.10$) to obtain a higher *ZT* value by decreasing the lattice thermal conductivity.

## Experimental Procedure

A series of samples were synthesized at the compositions of $FeV_{0.955-x}Hf_{0.045}Ti_xSb$ ($0 \leq x \leq 0.10$) by using the induction melting method under argon atmosphere. Then the ingot was crushed into powder and re-melted by arc melting at least 2 times under argon atmosphere. The prepared ingot was annealed at 700 $^0$C for 3 days in vacuum. Finally, the obtained ingots were crushed into powders and sintered into bulk by means of Hot Press technique with an applied pressure of 54 MPa at 600 $^0$C for 15 hours. The thermal conductivity $\kappa$ was measured by laser flash method, the Seebeck coefficient *S* by steady state method, and the electrical resistivity $\rho$ by four-probes method, over the wide temperature range of 300-700 K.

## Results

All the prepared samples contained the HH-phase as the dominant phase. We found that all the $FeV_{0.955-x}Hf_{0.045}Ti_xSb$ HH-phases showed a p-type behavior at $x > 0$. Remarkably, the $FeV_{0.905}Hf_{0.045}Ti_{0.05}Sb$ sample exhibited a large magnitude of Seebeck coefficient exceeding 300 $\mu VK^{-1}$ and a low electrical resistivity below 1.63 mΩ cm at 700 K. The lattice thermal conductivity $\kappa_{lat}$ of samples monotonically decreased with increasing Ti concentration at $0.025 < x < 0.075$. The $FeV_{0.88}Hf_{0.045}Ti_{0.075}Sb$ sample showed the minimal value of $\kappa_{tot} = 3.2$ W m$^{-1}$ K$^{-1}$ at 700 K.

As a result, the magnitude of *ZT* increased up to 1.15 at 700 K for $FeV_{0.905}Hf_{0.045}Ti_{0.05}Sb$. This *ZT* value is almost twice than that of $FeV_{0.80}Ti_{0.20}Sb$ ($ZT = 0.63$) previously reported (2).

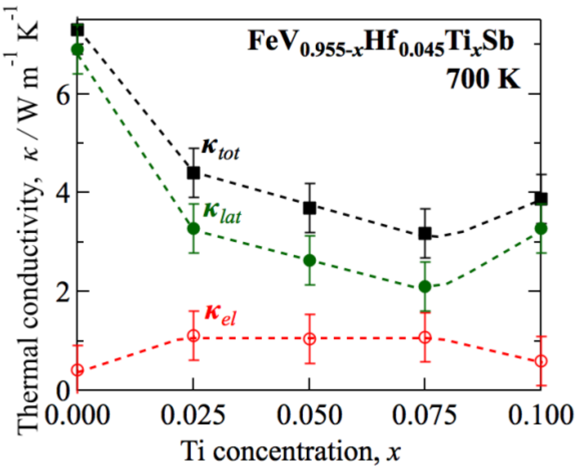


**Figure 1** Lattice thermal conductivity $\kappa_{lat}$, electron thermal conductivity $\kappa_{el}$ and total thermal conductivity $\kappa_{tot}$ of $FeV_{0.955-x}Hf_{0.045}Ti_xSb$ HH-phases at 700 K.

## Summary

We succeeded in effectively decreasing the lattice thermal conductivity of $FeV_{0.955-x}Hf_{0.045}Ti_xSb$ HH-phases without the degradation of its electrical properties to obtain a large *ZT*-value exceeding unity.

## References

[1] A. Yamamoto, T. Takeuchi: *J. Electron. Mater* **46**, 3200 (2016).
[2] K. Delime-Codrin *et al*, *Jpn. J. Appl. Phys* **56** , 111202 (2017).
[3] Fu C. *et al*, *J. Appl. Phys* **112**, 124915 (2012).