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Effect of Ti Substitution on Thermoelectric Properties of W-Doped Heusler Fe_2VAl Alloy

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Effects of element substitutions on thermoelectric properties of Heusler Fe_2VAl alloys were evaluated. By W substitution at the V site, the thermal conductivity is reduced effectively because of the enhancement of phonon scattering resulting from the introduction of W atoms, which have much greater atomic mass and volume than the constituent elements of Fe_2VAl alloy. W substitution is also effective to obtain a large negative Seebeck coefficient and high electrical conductivity through an electron injection effect. To change the conduction type from *n*-type to *p*-type, additional Ti substitution at the V site, which reduces the valence electron density, was examined. A positive Seebeck coefficient as high as that of conventional *p*-type Fe_2VAl alloy was obtained using a sufficient amount of Ti substitution. Electrical resistivity was reduced by the hole doping effect of the Ti substitution while maintaining low thermal conductivity. Compared with the conventional solo-Ti-substituted *p*-type Fe_2VAl alloy, the *ZT* value was improved, reaching 0.13 at 450 K.

Key words: Thermoelectric material, Heusler alloy, powder metallurgy, element substitution

INTRODUCTION

Thermoelectric devices have recently attracted renewed interest for their potential application in clean energy conversion systems. In particular, thermoelectric power generation is expected to play an important role in energy recovery from the vast amounts of waste heat to enhance energy utilization efficiency. The conversion efficiency of a thermoelectric device depends mainly on the material's thermoelectric properties, which are evaluated using the thermoelectric figure of merit $Z = S^2/\rho\kappa$, where S is the Seebeck coefficient, ρ is the electrical resistivity, and κ is the thermal conductivity. In addition, the power generation capability of a material under a certain temperature difference can be estimated using the thermoelectric power factor $PF = S^2/\rho$.

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A Heusler alloy, Fe_2VAl, is a promising candidate for thermoelectric power generation near room temperature because of its high PF value.[1–7] In the Fe_2VAl system, the high PF, resulting from the coexistence of a large S and low ρ, is reportedly produced by a steep pseudogap at the Fermi level.[2,3] Based on theoretical considerations, the sharply rising density of states enhances S according to Mott's theory.[8] The narrow pseudogap and residual density of states support the high electrical conductivity. The high PF value of 5.4 mW/mK^2 at 300 K has been confirmed experimentally.[1] In addition, the conduction type of this alloy can be controlled by adjustment of the valence electron density. For instance, *n*-type and *p*-type Fe_2VAl alloy are obtainable, respectively, by partial element substitution of Si at the Al site and Ti at the V site.[1,6] Therefore, a thermoelectric module consisting solely of the Fe_2VAl system can be fabricated.[9]

From a practical perspective, because of its high mechanical strength and excellent resistance to