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ACCEPTED MANUSCRIPT

Preparation and Thermoelectric Properties of Pseudogap Intermetallic (Ti_{1-x}V_x)NiSi Solid

Solutions

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Abstract

We theoretically and experimentally investigated the thermoelectric (TE) properties of TiNiSi-based

solid solutions with a pseudogap at the Fermi level in the electronic band structure. Calculation of

the TE properties of TiNiSi predicted that electron doping of TiNiSi leads to a higher power factor

than hole doping. According to this prediction, we prepared the partially V-substituted TiNiSi-based

compounds $(Ti_{1-x}V_x)NiSi$ (x = 0, 0.05, 0.10, 0.15, and 0.20) using arc-melting and subsequent spark

plasma sintering. An increase in the V content x improved the n-type TE properties: the absolute

values of the Seebeck coefficient and electrical conductivity both increased, while the thermal

conductivity slightly decreased. The highest dimensionless figure-of-merit, zT, was 0.032 at 600 K,

obtained for the x = 0.20 sample.

Keywords: TiNiSi-type compound; thermoelectric property; pseudogap; electronic structure

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1. Introduction

Thermoelectric (TE) conversion technologies have recently attracted much attention as potential

clean energy harvesting techniques because heat energy is directly converted into electricity using

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