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Thermoelectric Properties of $Yb_{1-x}(Er,Lu)_xAl_3$ Solid Solutions

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Ytterbium trialuminide ($YbAl_3$) has one of the largest thermoelectric power factors of known materials below room temperature, making it a material of interest for low-temperature thermoelectric devices. However, the high thermal conductivity, which is due to a combination of a large electronic thermal conductivity and a moderately large lattice thermal conductivity, is detrimental to the figure of merit. Substitution of different atoms on the Yb site was performed in order to assess their ability to favorably alter the electronic structure and/or reduce the lattice thermal conductivity. We have synthesized and studied the thermoelectric properties of the solid solutions of $YbAl_3$ with $ErAl_3$ and $LuAl_3$. Results for electrical conductivity, thermal conductivity, and Seebeck coefficient for several of these solid solutions over the temperature range of 80 K to 300 K are reported. Although most substituted samples are driven toward a metallic state, we find that for some compositions the figure of merit is enhanced relative to pure $YbAl_3$.

Key words: $YbAl_3$, trialuminides, thermoelectric properties

INTRODUCTION

Thermoelectric materials have the ability to convert directly between electrical and thermal energy; therefore, these materials are widely desired for applications such as waste heat recovery and solid-state cooling. The low efficiency of these materials has prevented widespread use, thus research is ongoing to find high-efficiency thermoelectric materials. The figure of merit z is the measure of the capability of a material to function as a thermoelectric, and is defined as $z = S^2\sigma/\kappa$, where S is the Seebeck coefficient, σ is the electrical conductivity, and κ is the thermal conductivity. The dimensionless figure of merit, zT, where T is the operating temperature, is generally used as a measure of the thermoelectric performance of a particular material.

Although thermoelectric materials are typically semiconductors, it has been shown that some intermediate valence compounds, such as ytterbium trialuminide ($YbAl_3$) and $CePd_3$, exhibit good thermoelectric properties.[1] This behavior is thought to arise due to the proximity of the f-electron level to the Fermi energy, resulting in a sharp feature in the electron density of states that gives rise to large Seebeck coefficient.[2,3] In the compound $YbAl_3$, it has been shown, through a combination of x-ray absorption,[4] photoemission,[5–7] and susceptibility[8–10] studies, that the Yb ion is in an intermediate valent state. Studies on single crystals[11–13] showed resistivity with magnitude typical of that of a metal, but unusually strong temperature dependence; additionally, Seebeck coefficients approaching $-100\ \mu V\ K^{-1}$ at room temperature have been observed.[11] Most of the experimental studies on this compound were performed on small single crystals grown using an Al flux.[14] The flux growth was necessary in order to suppress the formation of $YbAl_2$. Rowe et al.[15,16] reported the synthesis and thermoelectric properties of hot-pressed specimens of $YbAl_3$, synthesized by grinding single-crystal material with subsequent pressing. These samples exhibited larger resistivity than single crystals, but still exhibited thermoelectric power factors, $S^2\sigma$, near room temperature as much as three to four times that of Bi_2Te_3 at room temperature. However, in all cases, the zT of this material is still small due to the large thermal conductivity. The large thermal conductivity is due to a combination of

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