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Effect of Fe Substitution on Thermoelectric Properties of $Fe_xIn_{4-x}Se_3$ Compounds

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Starting from elemental powder mixtures of $Fe_xIn_{4-x}Se_3$ (x = 0, 0.05, 0.1, 0.15), polycrystalline In_4Se_3-based compounds with homogeneous microstructures were prepared by mechanical alloying (MA) and hot pressing (HP). With the increase of x from 0 to 0.15, the electrical resistivity and the absolute value of the Seebeck coefficient increased, while the thermal conductivity first decreased and then increased. The maximal dimensionless figure of merit ZT of 0.44 was obtained for the $Fe_xIn_{4-x}Se_3$ (x = 0.05) sample at 723 K.

Key words: In_4Se_3, MA-HP, Fe substitution, thermoelectric properties

INTRODUCTION

Because of their potential applications for direct thermal–electrical energy conversion and power generation,[1–4] interest in thermoelectric materials is continually growing. The performance of a material for thermoelectric application is characterized by the dimensionless figure of merit $ZT = S^2\sigma T/\kappa$, where S is the Seebeck coefficient, σ is the electrical conductivity, κ is the thermal conductivity, and T is the absolute temperature. Therefore, excellent thermoelectric materials should combine a high power factor $S^2\sigma$ with a low thermal conductivity κ.[5–7]

The In_4Se_3 compound has a layered structure, in which the layers are held together by weak van der Waals forces along the a axis with strong covalent bonding within the layer (b–c plane). A remarkably high ZT of 1.48 had been reported by Rhyee et al.[8] in the b–c plane of $In_4Se_{2.35}$ bulk single crystals. Peierls distortion and the resulting charge density wave (CDW) were thought to be the main causes of these excellent thermoelectric properties. Similar to the layered Bi_2Te_3-based thermoelectric materials,[9–12] In_4Se_3 single crystals are also unfavorable for further mechanical processing owing to their weak van der Waals bonding. Furthermore, the anisotropy of the transport properties of In_4Se_{3-x} single crystals is very notable; the ZT value in the a–b plane is much smaller, only about 0.5 at the same temperature.[8] Thus, polycrystalline In_4Se_3 compounds have attracted attention from researchers.[13–16] Recently, a very high thermoelectric performance of ZT about 1 was obtained at 700 K for this material.[15,16]

Except for self-doping (Se deficiency control), other element doping, such as Se site substitution,[17,18] has already been proved to be an available approach to promote the thermoelectric properties. However, less work had been reported about the effect of In site substitution of In_4Se_3-based compounds yet.[19] In fact, more work about cationic doping can help to understand the transport properties of In_4Se_3 compounds more comprehensively. In this work, a series of iron-doped $Fe_xIn_{4-x}Se_3$ (x = 0, 0.05, 0.1, 0.15) compounds were prepared by the MA-HP method, and the effect of Fe doping on the thermoelectric properties of the compounds is investigated and reported in this paper.

EXPERIMENTAL PROCEDURES

Elemental powders of In (100 mesh, 99.99 wt.%), Se (100 mesh, >99.9 wt.%), and Fe (200 mesh,

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