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A Review on Heusler Based Thermoelectric materials

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Abstract-

Thermoelectric technology is the conversion of temperature difference into electricity and its vive versa. In thermoelectric field, Heusler based materials have numerous advantages over other materials. Half-Heusler (HH) materials have mechanical as well as thermal stability at higher temperatures. Half Heusler based materials exhibit remarkable performance in the field of thermoelectrics. Here, significant advanced results of Heusler class of materials have been reviewed. Here, two approaches on Heusler based materials have been described i.e. reducing grain of Heusler materials and nanoinclusion in the Heusler matrix. As a result of these approaches, Heusler materials have performed key role in the thermoelectric field.

1. Introduction-

Thermoelectric (TE) materials have gained significant interest due to the direct conversion of heat into electricity and vice-versa[1]. They have been used for power generation applications as well as refrigeration purposes. The thermoelectric performance of materials has been evaluated by the dimensionless parameter i.e. $ZT = \frac{\alpha^2 \sigma T}{k_e + k_l}$, where α, σ, T, k_e, and k_l are Seebeck coefficient, electrical conductivity, temperature, electronic thermal conductivity, and lattice thermal conductivity respectively. In order to obtain high ZT, high power factor ($\alpha^2\sigma$) and low thermal conductivity (k=$k_e + k_l$) is required. However, due to the theclose interrelationship between these thermoelectric parameters, it is quite difficult to simultaneously optimize the electronic and thermal parameters[2].

Among different classes of materials, half–Heusler based materials have shown promising features. There are some excellent reviews available for HH thermoelectric materials[3,4].Hohl et al.[5]have reported that alloying at M site in MNiSn based material produce additional phonon scattering due to mass difference between dopant and host atom, consequently achieved thermal conductivity to 3.6-4.9 W/mK at room temperature. Uher et al.[6]showedSb doping at Sn site in $Zr_{0.5}Hf_{0.5}NiSn$ composition and obtained thermal conductivity 6.6 W/mK at room temperature. S. Sakurada et al. [7]achieved a low thermal conductivity 3W/mK for the Ti substituted $Zr_{0.25}Hf_{0.25}Ti_{0.5}NiSn$ due to mass fluctuation and further obtained ZT of 1.5 at 700K for Sb substituted $Zr_{0.25}Hf_{0.25}Ti_{0.5}NiSn_{0.998}Sb_{0.002}$ via optimization of power factor. Further M. Gurth et al.[8]achieved a ZT=1.2 at 800K for Hf free composition $Ti_{0.5}Zr_{0.5}NiSn_{0.98}Sb_{0.02}$. For p-type MCoSb, substitution of Sn optimizes carrier concentration and further via tuning of Hf to Ti ratio reduces thermal conductivity, achieved ZT=1.2 at 983K for $Ti_{0.25}Hf_{0.75}CoSb_{0.85}Sn_{0.15}$. C. Hu[9] et al. optimized the carrier concentration and achieved a high power factor 3×10^{-3} $Wm^{-1}K^{-2}$ at 800 K producing a ZT of 0.93 at 1123K.

Another p-type promising HH material FeNbSb exhibitsa high power factor and the main focus has been going on for reducing its high thermal conductivity. For instance, C. Fu et al. [10]have been able to achieve a high ZT value of 1.1 in $FeNb_{0.8}Ti_{0.2}Sb$ composition at 1100K via a band engineering approach. Junjie Yu et al[11] reduced the thermal conductivity by isoelectronic substitution, and a ZT_{max} value of ∼1.6 was obtained at 1200 K for the $Nb_{0.48}Ta_{0.32}Ti_{0.2}FeSb$ composition. Following this, we will discuss the various approaches implemented in HH compounds.

2. Recent approaches on HH materials-

2.1. Reducing grain size of HH materials-

Following these strategies, there are numerous experimental and theoretical findings. For instance,Giri Joshi et al[12] used the nanocomposite approach in n-type HH material to enhance the ZT value. The enhancement in ZT was mainly attributed to the reduction in thermal conductivity via increased phonon scattering due to the reduction in average grain size. Although enhancement in seeback coefficient was shown due to electron energy filtering effect but power factor was almost same compared to bulk counterpart. Finally ZT was boosted to 1 at 600-700C as compare to 0.8 for bulk material. Similarly reducing grain size in p-type also helped to increase the ZT value and peak ZT was enhanced from 0.5 for bulk to 0.8 for nanostructured material at 700C. In this case, there was a simultaneous increase in power factor because of enhanced seeback coefficient and reduction in thermal conductivity reaching 3.4 $Wm^{-1}K^{-1}$. However in both cases, average grain size was around 200nm after hot pressing. Therefore significant growth in grains was occured after hot pressing of ball milled powders and causes a limitation. Both the authors stated if grain size can be made around 10-50 nm, a more decrease in thermal conductivity can take place and can further enhance the ZT value. Thus reducing grain size can have significant effect on thermal conductivity, thermopower and can improve the figure of merit[13].

J.P.A. Makongo et al.[14]established the atomic scale structural engineering of thermoelectric (ASSET) for n-type HH material. The excess nickel was added in the composition $Zr_{0.25}Hf_{0.75}NiSn$ in order to in-situ synthesize Full Heusler inclusion with in the HH matrix. The FH concentration was controlled by adding appropriate excess nickel. As a result, seeback coefficient increased due to electron energy filtering effect via decreased carrier concentration at room temperature. However, increased mobility compensated the decrease in carrier concentration and finally electrical conductivity increased instead of decreasing. Further, moderate reduction in thermal conductivity via ASSET approach combined with increase in power factor boosted to a high ZT value. Following this, P. Sahoo et al.[15] developed the HH/FH nanocomposites for p-type HH material having composition $Ti_{0.5}Hf_{0.5}Co_{1+x}Sb_{0.9}Sn_{0.1}$. The results showed a large enhancement in seeback coefficient and small reduction in electrical conductivity leading to increased power factor. Here effect on thermal conductivity is not much incorporated. Amanbhardwaj et al.[16]achieved a ZT of 0.96 at 773 K for composition $Zr_{0.7}Hf_{0.3}Ni_{1.03}Sn$ as compare to ZT of 0.27 at 773K for normal HH $Zr_{0.7}Hf_{0.3}NiSn$. The enhancement in ZT was manifested by electron filtering, electron injection effect and phonon scattering mechanisms such as point defect scattering, alloy scattering and grain boundary scattering.Y. C.S. Birket et al[17] produced a ZT of 0.6 at around 800K by formation of secondary FH phase. These composites have shown decreased thermal conductivity because of effectively scattering of phonons due to irregular microstructure. Thus nanocomposites based on HH/FH can be an effective paradigm for improvement in ZT for Heusler thermoelectric materials.

2.2Nanoinclusion in the HH matrix-

W.J. Xie et al[18] have in-situ developed InSb inclusion in HH matrix. The size of inclusion was controlled by varying the amount of In and Sb in starting materials. The seebeck coefficient and electrical conductivity was enhanced by the electron filtering and electron injection phenomena respectively. Usually, InSb inclusion provided high mobility electrons to the matrix and as a result high electrical conductivity was maintained despite being reduced carrier concentration. Thermal conductivity also showed reduction due to phonon scattering at matrix-nanoinclusion interfaces. As a result all the three parameters were simultaneously optimized and ZT was elevated to 0.5 at 820K for 1% InSb inclusion in composition $Ti_{0.5}Zr_{0.25}Hf_{0.25}Co_{0.95}Ni_{0.05}Sb$ which was 160% greater than the material without inclusion. The InSb inclusion size was 10-30 nm for 1% InSb and further increment in size of inclusion deteriorated the thermoelectric properties. The same approach was also implemented by in-situ developing InSb inclusion on p-type [19]$TiCo_{0.85}Fe_{0.15}Sb$ and thermoelectric parameters are decoupled simultaneously. As a result with 1% InSbnanoinclusion in $TiCo_{0.85}Fe_{0.15}Sb$, ZT of 0.33 was obtained at 900K which was 450% greater than without inclusion matrix. A large number of HH materials with inclusion phase are developed and improved results are obtained.

3. Conclusion-

Conclusively, reducing grain size of Heusler materials as well as introducing nanoinclusion in the half-Heusler materials have been led to remarkable growth in thermoelectric figure of merit. These approaches led to the enhancement in ZT value via enhancing thermopower as well as reduction in thermal conductivity. Thus, this review introduce the important features of half-Heusler based materials.

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