페르미 면 형상제어에 따른 Bi-Sb-Te 이론 전자수송 특성 변화

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Impact of Fermi Surface Shape Engineering on Calculated Electronic Transport Properties of Bi-Sb-Te

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Abstract: Using thermoelectric refrigerators can address climate change because they do not utilize harmful greenhouse gases as refrigerants. To compete with current vapor compression cycle refrigerators, the thermoelectric performance of materials needs to be improved. However, improving thermoelectric performance is challenging because of the trade-off relationship between the Seebeck coefficient and electrical conductivity. Here, we demonstrate that decreasing conductivity effective mass by engineering the shape of the Fermi surface pocket (non-parabolicity factor) can decouple electrical conductivity from the Seebeck coefficient. The effect of engineering the non-parabolicity factor was shown by calculating the electronic transport properties of a state-of-the-art Bi-Sb-Te ingot via two-band model with varying non-parabolicity. The power factor (the product of the Seebeck coefficient squared and electrical conductivity) was calculated to be improved because of enhanced electrical conductivity, with an approximately constant Seebeck coefficient, using a non-parabolicity factor other than unity. Engineering the non-parabolicity factor to achieve lighter conductivity effective mass can improve the electronic transport properties of thermoelectric materials because it only improves electrical conductivity without decreasing the Seebeck coefficient (which is directly proportional to the band mass of a single Fermi surface pocket and not to the conductivity effective mass). Theoretically, it is demonstrated that a thermoelectric figure-of-merit zT higher than 1.3 can be achieved with a Bi-Sb-Te ingot if the non-parabolicity factor is engineered to be 0.2. Engineering the non-parabolicity factor is another effective band engineering approach, similar to band convergence, to achieve an effective improvement in power factor.

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Keywords: thermoelectric, non-parabolicity factor, power factor, conductivity effective mass, band mass of a single Fermi pocket

1. Introduction

Replacing current vapor-compression refrigerators with thermoelectric refrigerators can reduce the rate of climate

change. Unlike vapor-compression refrigerators, which utilize harmful greenhouse gases as refrigerants, thermoelectric refrigerators do not require any greenhouse gases to operate. Thermoelectric refrigerators can produce cooling using a two-dimensional array of alternating p - and n -type thermoelectric materials connected in series via the Peltier effect [1]. The efficiency of thermoelectric refrigerators depends on the performance of the thermoelectric materials, which is characterized by a dimensionless figure-of-merit, $zT = S^2\sigma T$

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κ , where S , σ , κ , and T are the Seebeck coefficient, electrical conductivity, thermal conductivity and the absolute temperature, respectively. However, currently the zT of known thermoelectric materials is not high enough to compete with vapor-compression refrigerators.

Considerable efforts have been devoted to improving zT . Band engineering is frequently adopted to maximize $S^2\sigma$ (power factor). Enhancing the power factor is challenging because of the trade-off between S and σ . If S is increased by making the band mass of a single Fermi surface pocket (m_b^*) heavier, the relevant σ will be decreased (band flattening). However, band convergence is an effective approach to enhance the power factor, as it enhances S (via increasing valley degeneracy (N_v) with a constant m_b^*) without deteriorating σ [2-4]. Identifying a band parameter that is not coupled to both S and σ is key to successful power factor improvement.

Although it has often been neglected to avoid complication, the types of band masses that determine S and σ are different. While S is directly proportional to the product of $N_v^{2/3}$ and m_b^* , which is equivalent to density-of-states effective mass ($m_d^* = N_v^{2/3} m_b^*$), σ is inversely proportional to conductivity effective mass (m_c^*) [5-7]. For a spherical Fermi surface pocket, its m_c^* is identical to m_b^* . However, for an ellipsoidal pocket, the m_c^* becomes smaller than the m_b^* [8]. Therefore, controlling Fermi surface nonparabolicity (K) can decouple σ from the S .

Here, we theoretically demonstrate that control of K is another effective band engineering approach to improve zT . The effects of engineering K on each of the electronic transport properties are calculated using a two-band model, where fitted band parameters of Bi-Sb-Te (the best candidate for thermoelectric refrigerators) are used. We find that K engineering enhances the power factor by increasing σ while keeping S constant.

2. Experimental Procedure

The two-band model (solutions of the Boltzmann transport equations) was fitted to the experimental S , and σ of a state-of-the-art p -type Bi-Sb-Te ingot measured as a function of T to obtain the band parameters (m_b^* and deformation potential, Ξ) of the valence and conduction bands in the Bi-Sb-Te (spherical Fermi surface pockets assumed) [9]. For 300 K,

0.3, and 0.6 m_e (electron rest mass) were adopted for m_b^* , corresponding to the valence and conduction bands, respectively. The N_v of both bands were set to be six, and an energy gap (E_g) of 0.19 eV was adopted in the two-band model [10-12]. It was assumed that acoustic phonon scattering limited the carrier mobility of both bands in the Bi-Sb-Te. Details on the two-band model fitting can be found in our previous works [4,13,14,15]. While keeping the aforementioned parameters (m_b^* , Ξ , N_v , and E_g) constant, electronic transport properties were calculated for different valence band K (= 0.2, 0.5, 1, 2.5, and 4) via the two-band model ($K = 1$ was assumed for the conduction band). Here, each electronic transport property was calculated as a function of the chemical carrier concentration (n) for $T = 300$ K. The effect of K engineering was evaluated by comparing the electronic transport properties calculated for $K \neq 1$ to those obtained for $K = 1$ (where Fermi surface pockets are spherical).

3. Results and Discussion

3.1. Decoupling m_c^* from m_b^* with $K \neq 1$

To theoretically demonstrate how changing the shape of Fermi surface pockets affects the thermoelectric performance of p -type Bi-Sb-Te, its electronic transport properties were calculated using varying valence band K with constant band parameters (m_b^* , Ξ , N_v , and E_g) under the acoustic phonon scattering assumption. The band parameters of Bi-Sb-Te were first obtained via the two-band model while assuming its Fermi surface pockets were spherical ($K = 1$ for both bands). The K is defined as a ratio of m_b^* along the longitudinal ellipsoid direction ($m_{b,\parallel}^*$) to that along the transverse ellipsoid direction ($m_{b,\perp}^*$).

$$K = \frac{m_{b,\parallel}^*}{m_{b,\perp}^*} \quad (1)$$

In terms of K , the degree of decoupling m_c^* from m_b^* is determined as below.

$$\frac{m_c^*}{m_b^*} = \frac{3K^{2/3}}{2K+1} \quad (2)$$

When K in Eq. (2) equals to unity, the m_c^* and m_b^* are identical, but for $K \neq 1$, the m_c^* becomes lighter than m_b^* as

Fig. 1. (a) Decoupling m_c^* from m_b^* as a function of K , (b) drift mobility (μ_d) as a function of n for different K at 300 K.

presented in Fig. 1(a) [8]. The solid black line in Fig. 1(a) represents m_c^*/m_b^* as a function of K . The symbols indicate m_c^*/m_b^* for each K in the range from 0.2 to 4. The specific K s were chosen so that their corresponding m_c^*/m_b^* ratios in the valence band were all different. Engineering K to be less than 1 ($m_{b,\parallel}^*$ being heavier than $m_{b,\perp}^*$) is more effective for decoupling m_c^* from m_b^* than changing K to be larger than 1, according to Fig. 1(a). In other words, decoupling σ from S becomes possible for a K other than 1.

The μ_d of Bi-Sb-Te was calculated as a function of n for varying valence band K (0.2, 0.5, 1, 2.5, and 4) to evaluate the effect of engineering K in drift mobility (μ_d) as shown in Fig. 1(b). Commonly, the μ_d was described to be inversely proportional to $m_b^{*5/2}$ assuming $K = 1$. However, the μ_d is more accurately described by a product of m_c^{*-1} and $m_b^{*-3/2}$ for $K \neq 1$, as given in Eq. (3).

$$\mu_d \propto \frac{1}{m_c^* \times m_b^{*3/2}} \quad (3)$$

If the m_c^* in Eq. (3) is expressed in terms of m_b^* and K (as in Eq. (2)), Eq. (3) becomes

$$\mu_d \propto \frac{1}{m_b^{*5/2}} \times \left(\frac{m_c^*}{m_b^*} \right)^{-1} = \frac{1}{m_b^{*5/2}} \times \left(\frac{2K+1}{3K^{2/3}} \right) \quad (4)$$

According to Eq. (4), the μ_d is inversely proportional to the m_c^*/m_b^* ratios, which depend on K (Fig. 1(a)). In Fig. 1(b), the μ_d calculated with $K = 1$ is the lowest for all ranges of n (green triangle and line). In contrast, the μ_d calculated with $K = 0.2$ is the highest (orange square and line). Because the m_c^*/m_b^* ratio for $K = 0.2$ ($m_c^*/m_b^* = 0.73$) is smaller than that for $K = 1$ ($m_c^*/m_b^* = 1$), the μ_d for $K = 0.2$ is calculated to be higher than that for $K = 1$. For other K , the corresponding μ_d also depends on the reciprocal of the m_c^*/m_b^* ratio (Eq. (4)). Therefore, a higher μ_d is expected with a K that gives a smaller m_c^*/m_b^* ratio.

Fig. 2. (a) σ , (b) electronic thermal conductivity (κ_e), and Lorenz number (L) in the inset of (b) calculated for different K as a function of n at 300 K.

3.2. Effect of varying m_c^*/m_b^* on σ via K engineering

To examine the effect of engineering K on σ , the σ of Bi-Sb-Te was calculated for varying valence band K (0.2 – 4), as shown in Fig. 2(a). Because the σ is directly proportional to μ_d as given below (e is the electric charge),

$$\sigma = ne\mu_d \quad (5)$$

a similar trend was observed in μ_d for different K (Fig. 1(b)), and this is also expected for σ . According to Fig. 2(a), σ for K other than unity were calculated to be higher than that for $K = 1$. Again, it is the value of m_c^*/m_b^* determined from a given K , and not the K itself that is correlated to σ . The m_c^*/m_b^* ratios which correspond to K (0.2 – 4) are provided in Table 1 (Eq. (2)).

From Table 1, the K arranged in order of decreasing m_c^*/m_b^* are: 1, 0.5, 2.5, 4, and 0.2. The calculated σ is also increased with decreasing m_c^*/m_b^* (K : 1 $\rightarrow$ 0.5 $\rightarrow$ 2.5 $\rightarrow$ 4 $\rightarrow$ 0.2) as shown in Fig. 2(a). Engineering K to reduce m_c^*/m_b^* was found to be beneficial to increase σ .

A minor difference between σ and μ_d is that σ only depends on m_c^* . Because n is directly proportional to $m_b^{*3/2}$, σ becomes inversely proportional to m_c^* only as below.

$$\sigma \propto n\mu_d \propto (m_b^{*3/2}) \left(\frac{1}{m_c^* \times m_b^{*3/2}} \right) = \frac{1}{m_c^*} \quad (6)$$

In other words, σ is the electronic transport parameter, which can be separated from S most effectively with relevant K engineering.

The effect of varying m_c^*/m_b^* (via K engineering) on electronic thermal conductivity (κ_e) was also studied. The heat-carrying carrier conduction (κ_e) contribute to the total κ along with heat conduction via lattice vibrations (lattice thermal conductivity, κ_l) and bipolar conduction (bipolar thermal conductivity, κ_{bp}) as in Eq. (7).

$$\kappa = \kappa_l + \kappa_e + \kappa_{bp} \quad (7)$$

Among κ_l , κ_e , and κ_{bp} , the κ_e is the most directly related to σ via the Wiedemann-Franz law, as below, where L is the Lorenz number [16].

$$\kappa_e = L\sigma T \quad (8)$$

Table 1. The m_c^*/m_b^* ratios and corresponding K .

m_c^*/m_b^*	K
1	1
0.94	0.5
0.92	2.5
0.83	4
0.73	0.2

This is because the L is independent of both m_b^* and m_c^* , the κ_e in Eq. (8) is directly proportional to σ at constant T . Therefore, a higher κ_e is expected with a K that corresponds to a lower m_c^*/m_b^* like σ , but the higher κ_e decreases zT . Fig. 2(b) shows the κ_e for varying K as a function of n . The κ_e with $K = 0.2$ (the lowest m_c^*/m_b^* , orange square and line) was calculated to be the largest, and that with $K = 1$ (the maximum m_c^*/m_b^* , green triangle, and line) was calculated to be the smallest. The inset in Fig. 2(b) shows the L calculated for varying K as a function of n . Because the L is not a function of m_c^* , the calculated L are all identical for different K . The discrepancy among κ_e for different K is calculated to increase at higher n . For the range of n where the thermoelectric performance of most materials is optimized ($\sim 10^{19} \text{ cm}^{-3}$), the increase in κ_e due to K engineering is negligible. Although decreasing m_c^*/m_b^* increases both κ_e and σ , the improvement in σ outweighs the increase in κ_e .

3.3. Effect of varying m_c^*/m_b^* on S via K engineering

To examine how varying m_c^*/m_b^* (via K engineering) affects S , the S of Bi-Sb-Te was calculated for varying valence band K (0.2 – 4) at 300 K, as shown in Fig. 3(a). The S for different K are almost identical for $n \geq \sim 5 \times 10^{18} \text{ cm}^{-3}$, but they are different for $n < \sim 5 \times 10^{18} \text{ cm}^{-3}$. Although S calculated from a single band is independent of m_c^* (but dependent on m_d^* instead), the overall S calculated from two bands does depend on m_c^* via σ contributions from each band. The overall S is calculated by Eq. (9) below, where S_i and σ_i are the partial contributions from each band ($i = \text{VB}$ (valence band), CB (conduction band)).

$$S = \frac{\sigma_{\text{VB}} S_{\text{VB}} + \sigma_{\text{CB}} S_{\text{CB}}}{\sigma_{\text{VB}} + \sigma_{\text{CB}}} \quad (9)$$

When σ_{VB} and σ_{CB} in Eq. (9) are comparable at low n , the

Fig. 3. (a) S , and (b) bipolar thermal conductivity (κ_{bp}) calculated for different K as a function of n at 300 K.

difference in σ_{VB} due to varying valence band K is well captured in the overall S . For example, the σ_{VB} for $K = 0.2$ is the highest among K in the range from 0.2 to 4 (Fig. 2(a)). Hence, the S for $K = 0.2$ is calculated to be the highest for $n < \sim 5 \times 10^{18}$ cm⁻³, as in Fig. 3(a) (S_{VB} , S_{CB} , and σ_{CB} being constant with respect to K). In Fig. 2(a), we simply stated that the overall σ increased because of the decrease in the m_c^*/m_b^* ratio. To be more specific, the increase in the overall σ was due to the increase in σ_{VB} originating from a decrease in the valence band m_c^*/m_b^* ratio (K of the conduction band was fixed). However, once the σ_{VB} becomes much greater than σ_{CB} at high n , the S in Eq. (9) converges to S_{VB} , as shown below.

$$S \approx \frac{\sigma_{VB} S_{VB}}{\sigma_{VB}} \approx S_{VB} \quad (10)$$

Because S_{VB} is independent of m_c^* , the S is calculated to be approximately invariant with respect to K at $n \geq \sim 5 \times 10^{18}$ cm⁻³, as in Fig. 3(a). Given that the optimum properties of thermoelectric materials are frequently realized at $n \sim 1 \times 10^{19}$ cm⁻³, it can be concluded that the S is not affected by varying K .

The effect of varying m_c^*/m_b^* (via K engineering) on κ_{bp} was also examined. Unlike κ_e , both S_i and σ_i ($i = VB, CB$) are required to calculate κ_{bp} , as shown below.

$$\kappa_{bp} = \frac{\sigma_{VB} \sigma_{CB}}{\sigma_{VB} + \sigma_{CB}} (S_{VB} - S_{CB})^2 T \quad (11)$$

In Eq. (11), the S_{VB} and S_{CB} are independent of varying K , as they do not depend on m_c^* . And because we assume that the K of the conduction band is unity for simplicity, only the

σ_{VB} is changed with varying K . Therefore, it is expected that the κ_{bp} with a low m_c^*/m_b^* will be high because of high σ_{VB} , as in the case of S . However as calculated in Fig. 3(b), the discrepancy in κ_{bp} due to different K is negligible for all n . Hence, varying K does not affect κ_{bp} .

3.4. Effect of varying m_c^*/m_b^* on power factor via K engineering

To demonstrate the effect of varying m_c^*/m_b^* (via K engineering) on the power factor, the power factor of Bi-Sb-Te was calculated for varying valence band K (0.2 – 4) at 300 K as shown in Fig. 4(a). Since suppressing m_c^*/m_b^* is beneficial to σ (Fig. 2(a)), while causing a negligible change in S (Fig. 3(a)), an improvement in the power factor is expected. According to Fig. 4(a), the highest power factor was calculated for the $K = 0.2$ (orange square and line), which corresponds to the lowest m_c^*/m_b^* (Table 1), and the lowest power factor was calculated for $K = 1$ (green triangle and line) which corresponds to the maximum m_c^*/m_b^* . The calculated power factor increased with decreasing m_c^*/m_b^* ($K: 1 \rightarrow 0.5 \rightarrow 2.5 \rightarrow 4 \rightarrow 0.2$), as observed in σ in Fig. 2(a). Therefore, engineering K to be other than unity will always improve the power factor.

Lastly, to investigate the effect of varying m_c^*/m_b^* (via K engineering) on zT , the zT of Bi-Sb-Te was calculated for varying valence band K (0.2 – 4) at 300 K as shown in Fig. 4(b). For the zT calculation, κ_l is required in addition to the κ_e and κ_{bp} calculated in Fig. 2(b) and 3(b), respectively. Because the κ_l cannot be calculated using the two-band model, the experimental κ_l of a state-of-the-art Bi-Sb-Te

Fig. 4. (a) Power factor and (b) zT calculated for different K as a function of n at 300 K. κ_l of 0.8 W/m-K was employed for the zT calculation.

ingot was adopted from the literature ($\kappa_l = 0.8$ W/m-K at 300 K) [9]. The highest zT was calculated for $K = 0.2$ for all n , as shown in Fig. 4(b). Its optimum zT was achieved near $n \sim 10^{19}$ cm $^{-3}$. The sharp decrease in zT for $n > 10^{19}$ cm $^{-3}$ is attributed to the increasing κ_e and κ_{bp} at high n . This confirms that engineering K to decrease m_c^*/m_b^* is another effective approach to improve zT .

Engineering K is another effective band engineering approach to improve the power factor of thermoelectric materials. Making K other than unity decouples m_c^* from m_b^* , which enables us to break the trade-off between S and σ . As m_c^*/m_b^* decreases, σ is improved without deteriorating S . Although κ_e is also increased with decreasing m_c^*/m_b^* , the κ_e increase is negligible compared to the σ increase. Therefore, zT improvement is guaranteed if the m_c^*/m_b^* is reduced by engineering K .

We assumed that the K of both the valence and conduction bands were unity when obtaining the band parameters of the state-of-the-art Bi-Sb-Te ingot from the two-band model fitting. However, it has been reported that the valence band K of Bi-Sb-Te was optically determined to be approximately 2 [17]. Consequently, the determined band parameters of Bi-Sb-Te (m_b^* , Ξ) with $K = 1$ can be marginally different from what they should be (with $K = 2$). The discrepancy between the fitted Ξ and the actual Ξ will be higher than that expected between the fitted and actual m_b^* because K only affects m_c^* -related parameters. Nonetheless, the fact that engineering K improves power factor remains intact because the beneficial effect of decreasing m_c^*/m_b^* on power factor applies to any set of band parameters.

Both decreasing m_c^*/m_b^* by engineering K and decreasing Ξ have similar impacts on μ_d as the μ_d is inversely proportional to the product of Ξ^2 , m_c^* and $m_b^{*3/2}$. In addition, because S is independent of Ξ , the effect of suppressing Ξ on electronic transport properties is almost identical to the effect of engineering K on electronic transport properties. Therefore, an additional optical study that measures m_b^* at different principal axes is required to confirm that an improvement in power factor originates from K engineering.

No experimental approach to engineer only K has been suggested yet. Although alloying is known to alter K , it also changes other band parameters at the same time, making the evaluation of the effect of K change difficult [17]. As an alternative, materials with innately low m_c^*/m_b^* have been theoretically sought as potential candidates for new high-performance thermoelectric materials [18].

Although the effect of engineering K was investigated using narrow band gap Bi-Sb-Te, its effect will be even greater for large band gap materials since the potential increase in κ_{bp} due to K engineering will be minimized because of their substantially low κ_{bp} [19]. Moreover, since we know that K other than unity can significantly alter the electronic transport properties of thermoelectric materials, accurate K input (obtained via measurements or simulations) is important to accurately determine materials' band parameters via band modeling.

4. Conclusions

A new band engineering approach that by-passes the trade-

off between S and σ has been suggested. Engineering the shape of Fermi surface pockets (K , non-parabolicity factor) to be ellipsoidal was found to decouple conductivity effective mass (m_c^*) from the band mass of a single Fermi pocket (m_b^*). When K is engineered to lower the m_c^*/m_b^* ratio, the σ is calculated to increase while S remains constant. It was calculated that the thermoelectric figure-of-merit (zT) of a Bi-Sb-Te ingot can be improved to higher than 1.3 if the non-parabolicity factor is engineered to be 0.2. Although alloying is known to change K , it also simultaneously alters other band parameters. However, it is suspected that alloying, combined with carefully designed doping, might only change K so that it improves the power factor of materials effectively.

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