Size effect in thermoelectric power factor of nondegenerate and degenerate low-dimensional semiconductors

Nguyen T. Hung*a, Ahmad R. T. Nugrahaa, and Riichiro Saiota

*Department of Physics, Tohoku University, Sendai 980-8578, Japan

Abstract

Low-dimensional materials have been known to give high thermoelectric (TE) performance by reducing the confinement length of the materials. Recently, we have shown that the TE power factor of low-dimensional semiconductors depends not only on the confinement length, but also on the thermal de Broglie wavelength of electrons or holes [Phys. Rev. Lett. 117, 036602 (2016)], in which the calculation was performed by assuming the semiconductors to be nondegenerate, i.e., we approximated the Fermi energy to lie only within the energy band gap, or in other words, the low doping approximation. Now, in this work, we generalize the previous results considering the degenerate case, in which the Fermi energy can exist in the valence or conduction bands, thus enabling a full consideration of heavy doping. An analytical formula for the TE power factor is derived to describe the size effect in the power factor of the low-dimensional semiconductors. We find that for both nondegenerate and degenerate cases, the TE power factor is enhanced in one- and two-dimensional semiconductors when the confinement length is smaller than the thermal de Broglie wavelength of the semiconductors, with Fermi energy around top (bottom) of valence (conduction) band for the p-type (n-type) semiconductors.

Keywords: Thermoelectric power factor; low-dimensional semiconductors; confinement length effect; thermal de Broglie wavelength

1. Introduction

Solid-state thermoelectricity may play a key role in the future for renewable energy performance through conversion of heat to electricity [1]. A good thermoelectric (TE) material is characterized by how efficient the
electric power can be obtained for a given heat source. In the application where the heat source is essentially free of charge, such as solar heat or waste heat, the best performance of a TE device is achieved by operating at maximum thermoelectric power factor [2]. The power factor is defined as, \( PF = S^2/\sigma \), where \( S \) is the Seebeck coefficient and \( \sigma \) is the electrical conductivity. On the other hand, when heat source is expensive, such as fossil fuel combustion, the efficiency of the TE devices is important to reduce the cost of generating power [2]. Such efficiency is usually evaluated by the dimensionless figure of merit, \( ZT = (S^2\sigma/\kappa)T \), where \( \kappa \) is thermal conductivity and \( T \) is the average absolute temperature.

There are many strategies on engineering phonons to increase \( ZT \) over the past two decades. One way is by reducing \( \kappa \) from phonon scattering in low-dimensional materials or nanostructures. For example, experiments using Si nanowires have observed that \( \kappa \) can be reduced below the theoretical limit of bulk Si (0.99 W/mK) that gave \( ZT = 0.6 \) at room temperature [3]. Another way is by using semiconductors with intrinsically low \( \kappa \) due to the strong anharmonicity of chemical bonds. For example, SnSe was recently reported to achieve a high \( ZT \) along specific crystallographic directions due to a very low lattice thermal conductivities (\( \kappa < 0.4 \) W/mK at 923 K) [4]. However, although there have been significant efforts to improve \( ZT \) by reducing \( \kappa \), enhancement of the \( PF \) remains a challenge.

A seminal work by Hicks and Dresselhaus in 1993 predicted that a decrease in the confinement length \( L \), which is defined by the diameter in one-dimensional (1D) materials and the thickness in two-dimensional (2D) materials, could increase the \( PF \) [5]. Recently, we pointed out that not only \( L \) but also the thermal de Broglie wavelength of carriers, \( \Lambda \), is an important parameter that affects the enhancement of the TE power factor [6]. The \( PF \) of the 1D and 2D semiconductors is enhanced compared with their bulk three-dimensional (3D) state only when \( L \) is smaller than \( \Lambda \), which becomes the signature of the quantum size effect in thermoelectricity. However, our previous study was performed by considering that the low-dimensional semiconductors are nondegenerate, i.e. we approximated the Fermi energy to lie only within the energy band gap. Experimentally, the nondegenerate case corresponds to the low doping approximation. To consider heavy doping, it is important to optimize the \( PF \) of the degenerate semiconductor case, in which the Fermi energy can exist anywhere within the valence or conduction bands.

In this work, we will show that the interplay between \( L \) and \( \Lambda \) is, interestingly, still the very same requirement that defines the size effect in thermoelectricity even for the degenerate semiconductors. By comparing with previous study [6], we will discuss the contribution from the nondegenerate and degenerate semiconductors on the condition of maximizing the \( PF \).

2. Model

We apply the one-band model to solve the Boltzmann transport equation within the relaxation time approximation (RTA), from which we can obtain the Seebeck coefficient and the electrical conductivity. The justification for the one-band model and the RTA was already given in some earlier studies, which concluded that the model is accurate enough to predict the thermoelectric properties of low dimensional semiconductors, such as the semiconducting carbon nanotubes (s-SWNTs) [7], the Bi\textsubscript{2}Te\textsubscript{3} thin films [5], and the Bi nanowires [8]. The Seebeck coefficient and the electrical conductivity within the one-band model are given, respectively, by [6,7].

\[
S = -\frac{k_B}{q} \left[ \eta \frac{r + D/2 + 1}{r + D/2} \frac{F_{r+D/2}}{F_{r+D/2-1}} \right],
\]

and

\[
\sigma = \frac{4q^2 \tau_0 \langle m \rangle^{D/2-1} (k_B T)^{D/2} (r + D/2)}{D L^{3-D} (2\pi)^{D/2} \hbar^D \Gamma(D/2)} F_{r+D/2-1},
\]

(1)
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