



Frequency dependent figure-of-merit in cylindrical thermoelectric nanodevices



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ABSTRACT

We use a theoretical mesoscopic model accounting for memory and nonlocal effects in thermoelectricity in order to investigate how the figure-of-merit in cylindrical thermoelectric nanodevices is conditioned in frequency-dependent situations. Two different situations, regarding the relative values of the particles' mean-free path and the characteristic size of the system, are analyzed. It is shown that in both situations the performances of the thermoelectric devices are reduced. However, nonlocal effects may be used as an aiding tool to have less marked reductions in those performances.

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1. Introduction

Alternative power sources based on energy harvesting are promising candidates to substitute batteries due to their ability to extract unlimited power from the environment or secondary processes, as well as to attain fully autonomous systems without periodical human interventions. Due to the large amount of residual heat yielding from the current energy generation technology based on fossil fuels, thermoelectric energy harvesters have received special attention in recent years. Thermoelectric devices offer a very attractive source of energy since they do not have moving parts, create pollution, or make noise.

In practical applications, the definition of a “good thermoelectric device” is usually related to the dimensionless product ZT , with T being the operating temperature, and Z the so-called figure-of-merit, defined as

$$Z = \frac{\epsilon^2 \sigma_e}{\lambda} \quad (1)$$

wherein ϵ is the Seebeck coefficient, σ_e the electrical conductivity, and λ the total thermal conductivity.

In thermoelectric materials heat is carried both by phonons and by electrons, and by definition, in Eq. (1) the total thermal conductivity is such that

$$\lambda = \lambda_p + \lambda_e \quad (2)$$

with λ_p being the phonon contribution to the thermal conductivity, whereas λ_e means the electron contribution to it [1–3].

Since the higher ZT , the higher the efficiency of a thermoelectric device, in order to widen the applications of thermoelectric power generators, in the last decades there has been a tremendous amount of researches to improve the values of ZT beyond those of bulk materials, which show, instead, low efficiencies. However, ZT has remained approximately equal to 1 for the past several decades in the case of archetype materials at all temperature ranges. These materials include antimony (Sb_2Te_3) and bismuth tellurides (Bi_2Te_3) for room temperature applications, lead telluride (PbTe) at moderate temperatures, and silicon-germanium (SiGe) alloys at high temperatures.

One of the primary challenges in developing advanced thermoelectric materials is decoupling ϵ , σ_e and λ which are typically strongly interdependent in such a way that an increase in ϵ usually results in a decrease in σ_e , and a decrease in σ_e produces a decrease in the electronic contribution to λ , following from the Wiedemann–Franz law.

Indeed, if the characteristic dimension of the material (or the system) is shortened, the new variable of length scale also becomes available for the control of the materials' properties. In particular, as the system size decreases and approaches nanometer length scales, new opportunities are allowed to vary the aforementioned parameters quasi-independently. Nanomaterials, therefore, provide an interesting avenue to achieve this goal, for example, making nanocomposites, adding nanoparticles to a bulk material, or employing one-dimensional nanostructures [4,5]. Nanosystems offer the possibility of an additional control of the transport coefficients [6–9]. For instance, whenever the characteristic size of the system is comparable to the mean-free path (mfp) ℓ of the different heat carriers (phonons, electrons, holes, etc.) it is known that a thermal conductivity reduction can be realized over

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a wide temperature range, or the power factor can be increased at the same time by increasing ϵ more than σ_e is decreased [10,11].

Although from experimental evidences it is very clear the importance of using nanotechnologies in thermoelectricity, the search of a very good thermoelectric device is still far from its final solution. This principally because the physics at nanoscale still presents several dark points, as for instance the role played by memory, nonlocal and nonlinear effects [12,13,6,8,7].

In particular memory effects may drastically influence, for example, the behavior of nanodevices at high frequencies [14,15]. In fact, in the simplest description of relaxational effects in the bulk for phonon heat transport, the heat flux \mathbf{q} is given by the Maxwell–Cattaneo equation

$$\tau_p D_t \mathbf{q} + \mathbf{q} = -\lambda \nabla T \quad (3)$$

where τ is the relaxation time due to the resistive interactions (momentum not conserved) between the heat carriers, and the symbol D_t means the material derivative. The Fourier transform of this equation leads to an effective frequency-dependent thermal conductivity of the form

$$\lambda^{\text{eff}}(\omega) = \frac{\lambda}{1 + (\omega\tau_p)^2} \quad (4)$$

which points out that the higher the frequency ω , the smaller the thermal conductivity.

This result may be interesting for thermoelectric applications, since small values of the thermal conductivity could lead to an enhancement of Z , according to Eq. (1).

Indeed, the analysis and modelization of heat transport in nanosystems are more complex since it is also required to pay a special attention to the boundary conditions [3]. The interest on wall effects, related to phonon–wall interactions [16,17], recently surged with the synthesis of nanowires with rough walls [18,19]. Furthermore, in thermoelectricity, one has to monitor also the frequency behavior of other material functions. Therefore, in the present paper, from a phenomenological point of view, we explore the frequency dependence of Z in cylindrical nanowires in order to point out whether the performances of thermoelectric devices may be enhanced by coupling relaxational and nonlocal effects in high-frequencies situations, or not. It is important to note that the approach used in the present paper rests on a mesoscopic level, as our main aim is to provide a first rough (but simple to obtain) estimation of the response of a thermoelectric device in frequency-dependent situations. In this sense, the present analysis should be only viewed as a first step towards more detailed microscopic scrutinies.

The structure of the paper is the following. In Section 2 we introduce transport equations with relaxational and nonlocal effects in heat and electric transport. In Section 3 we derive the frequency-dependent behavior of the figure-of-merit by modeling the interactions of the different heat carriers with the boundaries. In Section 4 we draw the main conclusions.

2. Enhanced thermoelectric equations with relaxational and nonlocal effects

On microscopic grounds both electrons and phonons may be viewed as a free-particle gas in a box [20]. In nonequilibrium mechanics, the statistical behavior of a thermodynamic system far from its thermodynamic equilibrium is described through the Boltzmann transport equation (BTE), which in the relaxation-time approximation reads:

$$\partial_t f + \cdot \nabla_{\mathbf{r}} f + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}} f = -\frac{f - f_0}{\tau} \quad (5)$$

wherein the subscripts \mathbf{r} and \mathbf{v} in the nabla operators represent the variables of the gradient, i.e., they are the position and the velocity of a set of particles, respectively. Moreover, in Eq. (5) $f(\mathbf{r}; \mathbf{v}; t)$ is the probably-density function, f_0 represents the equilibrium distribution of the carriers, and $\tau(\mathbf{r}; \mathbf{k})$ is their relaxation time, \mathbf{k} being the wave vector of the particle. In the BTE, f_0 is given by the Bose–Einstein distribution function (BEDf) in the case of phonons, i.e.,

$$f_0 = (e^{\hbar\nu/k_B T} - 1)^{-1}$$

wherein $\hbar = h/(2\pi)$ with h being the Planck constant, ν is the angular frequency, and k_B is the Boltzmann constant. In the case of electrons, instead, f_0 is expressed by the Fermi–Dirac distribution function (FDdf), i.e.,

$$f_0 = (e^{(\epsilon_i - \mu_e)/k_B T} + 1)^{-1}$$

with ϵ_i being the energy of the single-particle state, and μ_e is the chemical potential.

Indeed, it is possible to find several situations, as for example whenever the quantities $(\epsilon_i - \mu_e)$ and $\hbar\nu$ are much larger than $k_B T$, in which one can ignore the ± 1 in the denominator of f_0 , in order that the BEDf and the FDdf reduce to the Boltzmann distribution function [20]. In these cases, on intuitively ground, the solution of the BTE both for phonons, and for electrons would lead to equations showing the same mathematical behavior.

Starting from these considerations and in accordance with the basic principles of Extended Irreversible Thermodynamics [7,6], in Refs. [21,3] the following generalized transport equations to describe heat and electric transport with thermoelectric coupling have been considered:

$$\tau_p D_t \mathbf{q}^{(p)} + \mathbf{q}^{(p)} = -\lambda_p \nabla T + \ell_p^2 (\nabla^2 \mathbf{q}^{(p)} + 2\nabla \nabla \cdot \mathbf{q}^{(p)}) \quad (6a)$$

$$\tau_e D_t \mathbf{q}^{(e)} + \mathbf{q}^{(e)} = -(\lambda_e + \epsilon \Pi \sigma_e) \nabla T + \ell_e^2 (\nabla^2 \mathbf{q}^{(e)} + 2\nabla \nabla \cdot \mathbf{q}^{(e)}) + \Pi \sigma_e \mathbf{E} \quad (6b)$$

$$\tau_e D_t \mathbf{i} + \mathbf{i} = \sigma_e (\mathbf{E} - \epsilon \nabla T) + \ell_e^2 (\nabla^2 \mathbf{i} + 2\nabla \nabla \cdot \mathbf{i}) \quad (6c)$$

In these equations \mathbf{i} is the electric-current density, \mathbf{E} is the electric field, and Π is the Peltier coefficient. The basic idea lying under these equations is that the local heat flux shows both a phonon contribution $\mathbf{q}^{(p)}$, and an electron contribution $\mathbf{q}^{(e)}$ in such a way that $\mathbf{q} = \mathbf{q}^{(p)} + \mathbf{q}^{(e)}$.

Referring the readers to Section 4 for more comments about Eqs. (6), here let us only comment about the different material functions included therein. In Eqs. (6) τ_p and τ_e represent, respectively, the relaxation time due to phonons interactions and that due to electrons interactions. In more detail, the relaxation time τ_p may be related to the resistive mechanisms between the different particles in such a way that, through the Matthiessen rule, it is given as

$$\tau_p^{-1} = \tau_u^{-1} + \tau_i^{-1} + \tau_d^{-1} + \tau_{p-w}^{-1} + \tau_{e-p}^{-1}$$

where τ_u is the relaxation time of umklapp-phonon collisions, τ_i the relaxation time of phonon-impurity collisions, τ_d the relaxation time of phonon-defect collisions, and τ_{e-p} is the electron-phonon scattering-time [22]. Similarly, the electron relaxation time τ_e may be defined as

$$\tau_e^{-1} = \tau_{e-e}^{-1} + \tau_{e-p}^{-1}$$

with τ_{e-e} being the electron–electron scattering-time [23,24]. In principle, in defining both τ_p and τ_e further relaxation times, accounting for the phonon–wall and electron–wall interactions, should be taken into account. In our approach these interactions will be introduced by means of suitable boundary conditions in Section 3.

Moreover, in Eq. (6a) ℓ_p means the mfp of phonons, which is related both to resistive, and to the normal scattering of phonons

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