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Recipe for optimizing a solid-state thermal rectifier

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ABSTRACT

A thermal rectifier, i.e. a device in which the magnitude of the heat flux depends on the sign of the temperature gradient, has potential application in thermal logic systems, memory devices, and for long-term seasonal thermal energy storage. There is yet no clear guide for designing working rectifiers based on binary material systems. We use the analytical solution for thermal rectification in such a binary system that considers the local temperature dependence of the thermal conductivity to identify combinations that produce reasonable rectification. Often, between 200 and 400 K, the thermal conductivity of solid materials can be approximated as a linear function of temperature, $\kappa = aT + b$. The best binary material combinations occur when b/a approaches $-T_{hot}$ for one material and $-T_{cold}$ for the other. Our results provide clarity for experimentalists regarding suitable combinations. Applying the method with a sample database shows that a Si-Ce system exhibits the largest rectification with $R = 1.61$ although, since Ce easily oxidizes in air, manufacturing a Si-Fused SiO_2 rectifier with $R = 1.37$ may be more reasonable. We show that contacts made to a binary rectifier for either characterization or integration into a device can negatively impact device performance.

1. Introduction

The near parallel formulations of Ohm's law [1] and Fourier's law in the early 1800s [2] have evolved differently. While solid-state diodes have facilitated ubiquitous electronic devices [3], the thermal counterpart of the electronic diode has not found practical use. Conceptually, a thermal rectifier is a device in which the magnitude of heat flux depends on the sign of the applied temperature gradient [4–8]. Potential applications of thermal rectification include thermal logic systems [6,9], thermal memory devices [10], thermal transistors [7,11], and long-term seasonal thermal energy storage [12], all of which can conceivably run on abundant waste heat.

Since the fabrication of a solid-state thermal diode in 1936 [13], investigators have primarily focused on analytical and numerical modeling [14–23] or molecular dynamic simulations [8,24–32] so that limited experimental work has been reported [13,33–37]. Experiments with nanoscale systems are constrained by a lack of fundamental knowledge and challenges while fabricating devices with necessary tolerances [38]. A similar limitation occurs at the macroscale through an absence of a clear roadmap for device advancement.

Thermal rectification can be induced by varying the local temperature dependence of the thermal conductivity in a one-dimensional bi-segment steady state system. The theoretical maximum for rectification, when thermal conductivity is a linear function of temperature is $R = |J_F/J_R| = 3$, where J_F and J_R respectively denote the heat flux in the forward F and reverse R directions [17]. We present a method to design a system that approaches this upper limit using available materials in the 200–400 K common device operating temperature range. The analytical expression for R is expressed in terms of the thermal conductivities $\kappa_{1,2}$ of the two materials and the segment lengths $L_{1,2}$ of the binary material system. Predictions of R enable the selection of appropriate binary material combinations from an existing database.

2. Methods

The necessary condition for rectification is that $\kappa(T, x)$ be a non-separable function of temperature T and location x. This is satisfied by a one-dimensional (1D) perfectly insulated bi-segment system with no interfacial thermal resistance and where $\kappa(T)$ for each material has a different temperature dependence [16]. Around

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room temperature, a linear relationship between κ and T is often a reasonable approximation for a broad range of materials and typically becomes more suitable as ΔT decreases. Thus, the thermal conductivity of each segment is $\kappa = aT + b$, where a and b are constants. The coefficients of determination r^2 for fits made to the experimental data used in this study [39], are presented in Table 1. The raw data is provided in the supplementary material. To optimize thermal rectification, materials with opposing signs for $d\kappa/dT$ must be combined [15]. Hence, in Table 1, materials are separated into group 1 and 2 based on the sign of $d\kappa/dT$ and are referred to as M_1 and M_2, respectively.

We define $\theta = (T - T_c)/(T_h - T_c)$ and $y = x/L$, where T_c and T_h denote the cold and hot boundary temperatures, and x and L are respectively the linear position and total length of the combined material system, as shown in Fig. 1. Thus, θ and y vary between 0 and 1, and the dimensionless heat equation assumes the form,

$$\frac{d}{dy}\left(\widehat{\kappa}_i \frac{d\theta}{dy}\right) = 0, \quad i = 1, 2, \tag{1}$$

where, $\widehat{\kappa}_i$ denotes the dimensionless thermal conductivity $\widehat{\kappa}_i = \widehat{a}_i\theta + \widehat{b}_i$ with $\widehat{a}_i = a_i(T_h - T_c)/\kappa_{ref}$ and $\widehat{b}_i = (b_i + a_i T_c)/\kappa_{ref}$. The subscript i distinguishes the two material segments. For ease, we let $\kappa_{ref} = 1\ \mathrm{Wm^{-1}K^{-1}}$. $\widehat{\kappa}_i$ is positive, i.e. $\widehat{\kappa}_i > 0$, so $\widehat{a}_i$ and $\widehat{b}_i$ are constrained by (1) $\widehat{a}_i > -\widehat{b}_i$, and (2) $\widehat{b}_i > 0$.

Since the system is in steady-state and the heat flux in each segment is equal,

$$\widehat{J}_F = -\frac{\int_0^{\theta_{int_F}} \widehat{\kappa}_1(\theta)d\theta}{\int_0^f dy} = -\frac{\int_{\theta_{int_F}}^1 \widehat{\kappa}_2(\theta)d\theta}{\int_f^1 dy} \tag{2}$$

where $\widehat{J}_F$ and θ_{int_F} respectively denote the dimensionless heat flux and interfacial temperature in the forward direction, and $0 \le f \le 1$ is the length fraction of M_1 compared with the combined length of the binary material system, as shown in Fig. 1(a). With $\widehat{J}_R$ as the heat flux, the direction of the temperature gradient changes and the integration boundaries in the numerator are switched. Hence,

$$R = \frac{\widehat{J}_{1F}}{\widehat{J}_{1R}} = \frac{\widehat{J}_{2F}}{\widehat{J}_{2R}} = \frac{\widehat{J}_{1F}}{\widehat{J}_{2R}} = \frac{\widehat{J}_{2F}}{\widehat{J}_{1R}}, \text{ or} \tag{3}$$

$$R = \frac{\int_0^{\theta_{int_F}} \widehat{\kappa}_1(\theta)d\theta}{\int_{\theta_{int_R}}^1 \widehat{\kappa}_1(\theta)d\theta} = \frac{\int_{\theta_{int_F}}^1 \widehat{\kappa}_2(\theta)d\theta}{\int_0^{\theta_{int_R}} \widehat{\kappa}_2(\theta)d\theta} = \frac{(1-f)\int_0^{\theta_{int_F}} \widehat{\kappa}_1(\theta)d\theta}{f\int_0^{\theta_{int_R}} \widehat{\kappa}_2(\theta)d\theta}$$
$$= \frac{f\int_{\theta_{int_F}}^1 \widehat{\kappa}_2(\theta)d\theta}{(1-f)\int_{\theta_{int_R}}^1 \widehat{\kappa}_1(\theta)d\theta}. \tag{4}$$

3. Results and discussion

Eq. (1) determines $\theta(y)$ and hence $\widehat{\kappa}(\theta)$. Either these two variables or Eq. (4) provides a solution for $R(\widehat{a}_1, \widehat{b}_1, \widehat{a}_2, \widehat{b}_2, f)$, hereinafter referred to as the *analytical solution*, which is included in appendix A. Eq. (4) is further simplified by noting that maximum rectification occurs when $\theta_{int_F} = \theta_{int_R} = \theta_{int}$ [17,36].

Fig. 1(b) presents the analytical solution for R for some example material combinations. The figure also reveals the sensitivity of R to f around its maximum value R_{max} (at f_{opt}). For example, $(f_{opt}, R_{max}) = (0.94, 1.61)$ for a Si-Ce binary system, which has the highest thermal rectification among the evaluated material combinations. The value of $|dR/df|$ is also large around R_{max}, indicating high sensitivity to f. This may make it experimentally challenging to achieve the highest thermal rectification due to the level of precision required while fabricating a device. The temperature profile for the Si-Ce system is presented in Fig. 1(c). By using $f = 0.94$ the system is optimized for R. Therefore, the intersection of the temperature profiles for $\widehat{J}_F$ and $\widehat{J}_R$ occurs at the interface of the two materials (f_{opt}). Since the interface temperature is unchanged for both forward and reverse flux cases, $\widehat{\kappa}_{1,2}(\theta_{int_F}) = \widehat{\kappa}_{1,2}(\theta_{int_R}) = \widehat{\kappa}_{1,2}(\theta_{int})$, as depicted in Fig. 1 (d).

Employing Eq. (4), R is determined from either $\widehat{\kappa}_1(\theta)$ and θ_{int}, or $\widehat{\kappa}_2(\theta)$ and θ_{int}. The properties that make a material ideal for thermal rectification are independent of its binary counterpart, i.e. M_1 can be selected without taking M_2 into account. The only link between the two materials is through θ_{int} since the secondary material influences the temperature profile and thus the interfacial temperature. The length fraction of each material can be tuned until the interface temperature reaches θ_{int} and hence R_{max} is achieved. By evaluating the integrals in Eq. (4) as shown in appendix B, R_{max} occurs when

$$\widehat{a}_1/\widehat{b}_1 \to -1 \text{ and } \widehat{a}_2/\widehat{b}_2 \to +\infty. \tag{5}$$

Table 1
Material database, their linear fit parameters to $\widehat{\kappa}(\theta)$, and their corresponding coefficients of determinations r^2, between 200 and 400 K [39]. The data are divided in two groups based on the sign of $d\widehat{\kappa}/d\theta$ which is determined by the sign of $\widehat{a}$. The codes are used to refer to various material combinations.

Group 1: $\frac{d\widehat{\kappa}}{d\theta} < 0$					Group 2: $\frac{d\widehat{\kappa}}{d\theta} > 0$				
Code	Material	$\widehat{a}_1$	$\widehat{b}_1$	r^2	Code	Material	$\widehat{a}_2$	$\widehat{b}_2$	r^2
1	Fe	−24.40	93.00	0.99	A	Fused SiO_2	0.36	1.18	0.96
2	BeO	−221.50	398.47	0.95	B	Ce	8.87	5.53	0.71
3	Bi	−2.87	10.81	0.94	C	Al	4.61	235.30	0.63
4	Ge	−52.12	90.06	0.94					
5	Single Crystal SiO_2	−8.47	15.29	0.94					
6	Cu	−20.45	410.10	0.93					
7	Si	−157.78	240.19	0.92					
8	Cu_2O	−2.00	7.27	0.91					
9	Al_2O_3	−46.69	73.70	0.90					
10	Au	−14.56	324.45	0.88					
11	Er	−0.54	14.49	0.69					