International Journal of Heat and Mass Transfer 97 (2016) 603–610

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Thermal rectifier efficiency of various bulk–nanoporous silicon devices

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ARTICLE INFO

Article history:
Received 24 November 2015
Received in revised form 17 February 2016
Accepted 17 February 2016
Available online 2 March 2016

Keywords:
Thermal rectifiers
Phononics
Bulk–nanoporous silicon
Homogeneous and non-homogeneous systems

ABSTRACT

Our objective is to calculate and to compare the rectifying thermal coefficient of various bulk–porous silicon configurations. We consider successively homogeneous devices involving two- and three elements and several graded devices characterized by variable porosity and/or size of the pores along the system. The criterion is to obtain rectifying coefficients different from one in order that thermal rectification be as efficient as possible. In that respect, it turns out that the porous–bulk–porous configurations are of little interest, in contrast to the bulk–porous–bulk systems whose rectifying coefficients may be larger than two and comparable to the values of the simpler two-element bulk–porous devices. Graded systems with either a variable porosity or a variable pore size do not exhibit better results. However, when both porosity and pore size are varying along the device, the highest efficiency is obtained.

1. Introduction

Thermal rectifiers have attracted an increased interest not only in fundamental but also in applied research, [1–6] presently framed within the relatively new topic of *phononics* [7–9]. The concept of thermal rectification can be traced back to Starr in 1936 [10]. By analogy with electronic diodes used for the control of electric current, thermal rectifiers are devices allowing heat to flow easily in one direction but offering strong resistance in the reverse direction. Search for suitable materials and configurations enhancing heat rectification has been intensely activated principally during the two last decades [11–14]. Among the current and widely used techniques, let us mention these based on adsorption/desorption properties [15], phase change [16], photon radiation [17], thermal expansion–contraction [6] and heat transfer between materials with different temperature-dependent heat conductivities [18,19], the main objective is the search for thermal diodes with the highest performance. The subject opens the way to specific applications, especially in the field of energy-saving structures, solar energy conversion, nano-electronic cooling, aero-spatial industry and cryogenics.

In the present theoretical approach, we consider successively discontinuous devices constituted by the junction of homogeneous bulk and nanoporous Si and porous non-homogenous Si. The purpose of this work is the search of suitable material configurations leading to the most efficient heat rectification. Although the actual analysis is limited to silicon there will be no difficulty to extend it to other materials.

The underlying property responsible for heat rectification is the behavior of the heat conductivity of nanoporous materials [1,20]. When the dimensions of the pores are comparable or smaller than the mean free path of the phonons, the effective heat conductivity of the porous material is generally much lower than that of the corresponding bulk crystal.

Thermal rectification in Si devices has been recently analyzed theoretically by Criado-Sancho et al. [1,20]. These authors base their approach on an expression of Fourier's law using for the effective heat conductivity an expression derived in the framework of phonon hydrodynamics. Our aim is to complement and compare with Criado-Sancho et al. results, proposing novel configurations with better results. The present analysis uses instead for the heat conductivity a relation proposed by Sumirat et al. [21], which emphasizes more particularly the effect of phonon scattering by pores. The Sumirat model has been validated with results derived by Machrafi and Lebon [22] in the framework of extended irreversible thermodynamics [23], it is mathematically simpler than the hydrodynamic model used by Criado et al. and allows for a more exhaustive exploration of several aspects of the problem.

In this paper, we investigate which configuration among several bulk–nanoporous lattices will yield the most efficient rectification. We will examine successively several different devices consisting of juxtaposed homogeneous bulk and nanoporous Si samples and

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http://dx.doi.org/10.1016/j.ijheatmasstransfer.2016.02.048
0017-9310/

Nomenclature

a_p	pore size
C	specific heat
k	heat conductivity
Kn	Knudsen number
L	length of the element
q	heat flux
R	rectifying coefficient
R_{th}	thermal boundary resistance
T	temperature
v	phonon group velocity
x	longitudinal coordinate

Greek symbols

φ	porosity
Λ	mean free path

Subscripts

d	direct direction
F	interface
G	interface
H	hot
i = 1, 2, 3	element under study
L	low
max	maximum
min	minimum
r	reverse direction
0	reference value

Superscripts

eff	effective
0	bulk

will end with non-homogeneous porous materials wherein both porosity and particles' size are varying in space.

The important quantity characterizing rectification is the thermal rectifying coefficient R (also called diodicity by some researchers) defined by the ratio of the heat flows in the direct and reverse directions:

$$R \equiv |q_d|/|q_r| \tag{1}$$

with q_d the heat current in the direct "conducting" direction and q_r in the reverse "insulating" one. To get an amplification effect, one must have $R \neq 1$; when $|q_d|$ is larger than $|q_r|$ (which is the situation investigated in the present work), one has $R > 1$. Of course, if the conducting and insulating directions would be switched, one should have $R < 1$. In two phase situations involving bulk and porous Si samples it was found [1] that R is of the order of 1.5, it is also noted that the effect of porosity on heat conduction is particularly relevant at low temperatures not exceeding 200 K. Similar values for R were obtained with two polycrystalline cobalt oxides segments [19], more recently, a solid state structure with shape memory alloys was built by Tso and Chao [4] who recorded an R-value of about 90.

The mechanism underlying thermal rectification has also been interpreted as a consequence of a negative differential thermal resistance defined as $R_H = (\partial q/\partial T_H)_{T_L}$ and an equivalent definition for R_L obtained by permuting the different indices H and L, H and L standing for hot and low temperature respectively. Classically, the heat flow increases with increasing thermal gradients and therefore both R_H and R_L are positive so that by defining R as $R = |R_L|/(|R_H| + |R_L|)$, it is found that $R < 1$ and the device will not work as a rectifier for which it is imperative that either R_L or R_H be negative. In the following, we will not follow this route. Instead, we will focus on the definition (1) of diodicity. This choice is not unique, though. For instance, some authors (e.g. [4,18]) use the following quantities to define the level of rectification, either

$$R^* = \frac{|q_d| - |q_r|}{|q_d| + |q_r|} = \frac{R-1}{R+1} \tag{2}$$

or

$$R^{**} = \frac{|q_d| - |q_r|}{|q_r|} = R - 1 \tag{3}$$

By selecting one or another of these definitions, one obtains values of the diodicity that may differ slightly as illustrated in Section 4.

The paper will run as follows. In Section 2, the effect of porosity on the effective thermal conductivity of nanoporous materials, illustrated by nanoporous Si, is discussed. In Section 3, thermal rectifiers consisting of homogeneous bulk–porous Si configurations are considered: two-phase bulk–porous Si and three-phase devices, namely bulk–porous–bulk Si and porous–bulk–porous Si systems, are successively examined. In Section 4, graded nanoporous Si systems, with the porosity and/or pore size varying gradually along the sample, are investigated. Conclusions are drawn in Section 5.

2. Thermal conductivity of bulk and porous silicon

The expression of the thermal conductivity of porous materials is a central quantity in the determination of the rectifying coefficient (see for instance [24] for a review). In the present analysis, we use for the effective thermal conductivity of porous Si the analytical approximate result derived by Sumirat et al. [21] on the bases of the kinetic theory of phonons in solids, namely

$$k^{eff}(\varphi, T, Kn) = k^0(T)\frac{(1-\varphi)}{1 + \sqrt[3]{\varphi}Kn(T)}. \tag{4}$$

This formula will be used as a mathematically simple efficient tool in order to perform our investigation. The quantity $k^0(T)$ is the bulk thermal conductivity, which depends generally on the temperature T. For Si, it is of the order 3700 W m^{-1} K^{-1} at 40 K, 2200 W m^{-1} K^{-1} at 58 K, 1350 W m^{-1} K^{-1} at 79 K, 800 W m^{-1} K^{-1} at 105 K, 560 W m^{-1} K^{-1} at 127 K, and 475 W m^{-1} K^{-1} at 153 K [10]. The behavior of the silicon bulk thermal conductivity versus the temperature in the range 40–150 K is given by the solid black line of Fig. 1. In relation (4), φ designates the porosity, i.e. the ratio

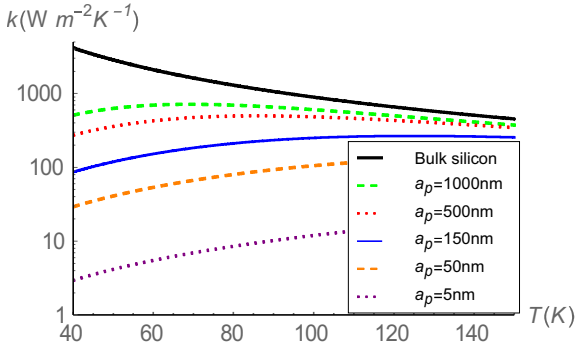

Fig. 1. Thermal conductivity versus temperature for bulk ($k^0(T)$) and nanoporous Si (Eq. (4)): porosity $\varphi = 0.1$ and pore sizes a_p are varying from 1000 to 5 nm.