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Abstract. Thermal diodes are devices that allow heat to flow preferentially in one direction. This unique thermal management capability has attracted attention in various applications, like electronics, sensors, energy conversion or space applications, among others. Despite their interest, the development of efficient thermal diodes remains still a challenge. In this paper, we report a scalable and adjustable thermal diode based on a multilayer structure that consists of a combination of phase change and phase invariant materials. We applied a parametric sweep in order to find the optimum conditions to maximize the thermal rectification ratio. Our simulations predicted a maximum thermal rectification ratio of ~20%. To evaluate the impact of these devices in real applications, we theoretically analysed the performance of a magnetocaloric refrigerating device that integrates this thermal diode. The results showed a 0.18 K temperature span between the heat source and the heat sink at an operating frequency of 25 Hz.

1. Introduction

Thermal diodes are devices that propagate heat preferentially in one direction. This leads to an asymmetric thermal transfer function, i.e. heat flux versus thermal bias.[1–3] These components have the potential to expand the capabilities of modern thermal management technology, like enhancing the temperature control in nanoelectronics,[4] increasing the power density in caloric refrigeration[5,6] or reducing the temperature fluctuations in space applications.[7] However, current thermal diodes are limited by their complex designs,[8] the lack of temperature tunability[9] or their limited thermal rectification control.[10] The performance of thermal diodes is defined as the rectification ratio (*RR*) between the forward (q''_{fwd}) and reverse (q''_{rev}) heat fluxes across the device. Assuming $q''_{fwd} > q''_{rev}$, the rectification ratio can be expressed mathematically as follows,

$$RR = \frac{|q''_{fwd}| - |q''_{rev}|}{|q''_{rev}|} \tag{1}$$

In the last few years, researchers have used different strategies to maximize the *RR* of these devices, e.g. shape-induced asymmetry or junctions of materials with different thermal properties.[2] In most of these approaches, a key aspect for an optimum thermal performance is related to the properties of the material.[11] In other words, materials that exhibit drastic changes in thermal conductivity with temperature are desired for developing thermal diodes. Phase change materials (PCM), whose thermal conductivity vary when the temperature is beyond the phase transition critical temperature (T_{crit}), are considered as ideal candidates. As an example, vanadium dioxide (VO_2) is one of the most famous PCMs that undergo a solid-to-solid phase transition at $T_{crit} \sim 340$ K.[12] This material has become popular to develop thermal diodes due to ~60% change in the thermal conductivity between phases.[7,9,12] As an example, Zhu *et al.*[9] presented a VO_2

based thermal diode with a maximal rectification ratio of 28 %. Additionally, PCMs can be combined with phase invariant materials (PIM), which presents a nearly uniform thermal conductivity within the PCM temperature range, to develop thermal diodes.[13] Kobayashi *et al.* [14] presented a thermal diode based on this concept by using the PCM MnV_2O_4 and the PIM $La_{1.98}Nd_{0.02}CuO_4$. In this paper, we analyzed a multilayer PCM/PIM structure for the realization of a versatile thermal diode. This functional structure offers numerous advantages over previously reported thermal diodes, including simple design, scalability, temperature tunability, easy integration into various applications and possibility of operation at the micro- and macro-scale. First, we carried out numerical investigations using finite element modelling to find the optimal PCM/PIM multilayer configuration that leads to high thermal rectification. Second, we theoretically analyzed the effect of integrating such type of thermal diodes in a magnetocaloric (MC) refrigeration device. In a further study we thoroughly analyzed the thermal rectification properties in a multilayer thermal diode structure by considering realistic material properties in the individual layers.[15]

2. Finite element model (FEM)

We carried out a parametric analysis using FEM to analyze the thermal rectification performance of a diode structure consisting of alternating layers of PCM and PIM. The length (L, x-direction) and the height (H, y-direction) of the diode was fixed to 1 µm, while a temperature gradient was applied between the two ends of the device (T_{hot} and T_{cold}). We fixed T_{cold} to 250 K and used different values for T_{hot}. Then, we varied the number (n) of PCM and PIM blocks and their thermal properties to achieve the maximum possible thermal rectification ratio. Table 1 presents the investigated parameter values of all considered properties. FEM (COMSOL® Multiphysics) heat transfer simulations were performed under steady state conditions using the classical Fourier's law equations. The heat flux density q'' [W/m²], i.e. sample width independent, was calculated both in the forward and reverse direction using the following equation,

$$q'' = -k \cdot \frac{\Delta T}{\Delta L} \quad (2)$$

where k is the thermal conductivity and ΔT the temperature span between the hot and the cold reservoir over ΔL, the length of the diode between the heat source and the heat sink. The RR was then calculated by using equation (1).

Table 1. Sweeping parameters and their investigated values

Parameter	Values
n	1, 2, 3
L [µm]	1
H [µm]	1
k_{PCM} [W/(m·K)]	1-1.5,5-7.5,10-15
k_{PIM} [W/(m·K)]	1, 10, 100
T_{hot} [K]	400, 700, 1000
T_{crit} [K]	300, 500, 700
T_{cold} [K]	250

3. Results

A maximum RR of ~20 % was observed for the PCM/PIM multilayer configuration presented in Fig. 1. Fig 1 a) and b) show the temperature in the forward and reverse direction. Fig 1 c) and d) show the thermal conductivity and temperature profile in the forward and reverse direction along the length of the structure. In this best case scenario, the following PIMs could be used: Si as PIM_1 and SiO_2 as PIM_2. For the PCMs we considered hypothetical materials that have solid-to-solid transitions near T_{crit} ~500 K with thermal conductivity values of: k_{min}=5 W/(m·K) *vs* k_{max}=7.5 W/(m·K). In the forward direction, the thermal conductivity of PIM_1 is high enough to keep both PCM blocks in their high thermally conductive states. In the reverse direction, the temperature gradient drops largely across PIM_2, which has a low thermal conductivity. This causes the temperature of the PCM_2 to become lower than T_{crit}. Therefore, under these circumstances, both PCMs are in their low thermally conductive states. Similar thermal rectification values were found at other temperatures ranges and material configurations (Table 1). The design parameters of the thermal diode, like temperature, PCMs or PIMs, size or geometry, can be adjusted depending on the application targeted. Further simulations showed that the *RR* can be greatly improved by using different thermal conductivity properties for the individual PCM blocks.

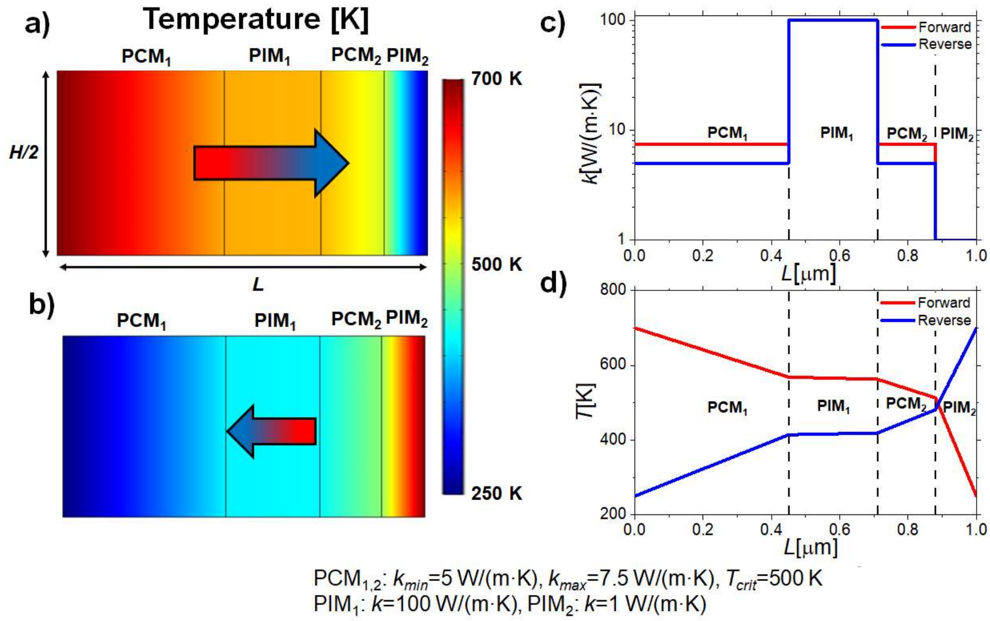

Figure 1. Forward vs reverse heat flow for the best-case scenario, achieving a RR_{max}=20 %: a) and b) show the temperature gradient in the forward and reverse direction. c) Thermal conductivity (*k*) and d) Temperature profile (*T*) in forward and reverse direction along the length of the structure.

4. Magnetocaloric (MC) refrigeration

The thermal diodes (TDs) described above can be used to improve the performance of MC devices.[5] For that reason, we analyzed theoretically the performance of one dimensional (1D) MC gadolinium device sandwiched between two TDs. Then, we determined the temperature span between the heat sink (HSI) and heat source (HSO). Fig. 2a illustrates the two configurations studied with their standard operating temperatures. The model included convective boundary conditions where the ambient temperature was held constant at 292.5 K. Table 2 shows the used parameters for the simulated MC device. For the material properties of the TDs, we considered hypothetical values. Under quasi-steady-state operation, the following temperature spans between the heat sink and heat source were obtained: 0.14 K at 15 Hz, 0.16 K at 20 Hz and 0.18 K at 25 Hz. The time evolution for 25 Hz is presented in Fig. 2b.

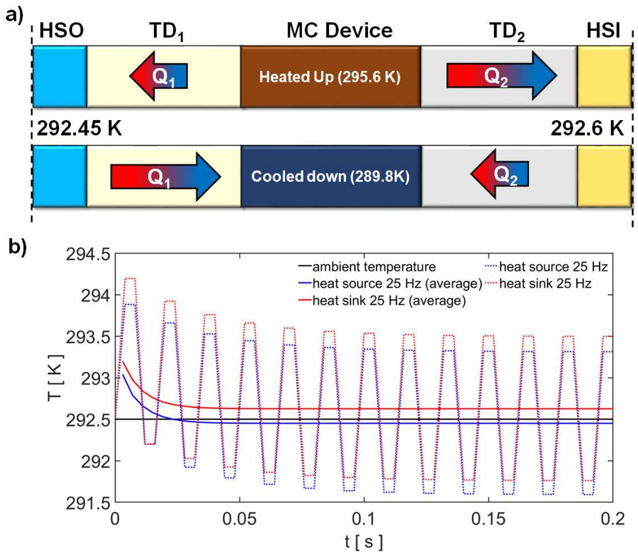

Figure 2. a) Schematic drawing of the MC device under two operating conditions. b) The established temperature span inside the 1D MC device at 25 Hz.

Table 2. Parameter of the MC device with gadolinium

Parameter	Values
L [μm]	9
H [μm]	1
k_{PCM1} [W/(m·K)]	1-0.1
k_{PCM2} [W/(m·K)]	1-0.01
k_{PIM1} [W/(m·K)]	100
k_{PIM2} [W/(m·K)]	1
Operating frequencies [Hz]	15, 20, 25
Operating magnetic field [T]	1
(De)Magnetization time [ms]	10
Intial MC T [K]	292.5

5. Conclusion and Prospects

The proposed PCM/PIM multilayer structure shows an approach for the development of highly efficient and tunable TDs. By chosing the appropriate PCM and PIM layers, this type of TD can be used in various applications. The thermal *RR* can be changed by adjusting different parameters, e.g. the thermal conductivity of the PCM and PIM layers, the length of the blocks or by considering asymetric geometries. Finally, we considered the operation of MC device under the presence of these TDs. The application in MC devices is especially interesting because it enables higher operating frequencies compared to the conventional active caloric regeneration process, increasing the cooling power and the possibility of building static solid-state caloric refrigerating devices.[5] Our TDs led to a 0.18 K temperature span between the heat source and the heat sink at the operating frequency of 25 Hz. The application of these devices is not only limited to caloric refrigeration but also,[15,16] they are bound to play a relevant role in other energy harvesting technologies.[7]

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