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Thermal rectification assisted by lattice transitions

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ABSTRACT

The most fundamental electronic device is the electrical diode; its thermal equivalent is the thermal diode, a device that conducts heat in only one direction. Currently used bulk and molecular mechanisms which can potentially result in thermal rectifying behavior have not evidenced that the rectification factor can reach an order of magnitude, which is an arbitrary limit required to deem the effect useful for engineered systems. Here we have succeeded in building thermal diodes with thermal rectification factors up to 1.47. Devices manipulate the heat flux via single-stage solid–solid transitions which promotes a change in the vibrational frequency of phonons at the transition temperature generating an asymmetric thermal conductance on the device. Thermal rectification effect is analyzed within the framework of the acoustic mismatch model, and the results show that the rectification factor can be further enhanced by accentuating the differences in acoustic properties between materials and by increasing the thermal bias. Furthermore, thermal diodes present a well-defined *breakdown* as well as *forward bias* temperatures given by the endothermic transition temperature during forward and reverse bias mode respectively which control accurately the *on state* of the device. This approach paves the way to pursuit the one order limit at room temperature in a simple way and opens a new route towards the next generation of thermal devices.

1. Introduction

Waste heat occurs in many areas of daily life because world's energy consumption is inefficient. In general, generating 1 W of power requires about 3 W of energy input and involves dumping into the environment the equivalent of about 2 W of power in the form of heat. Efficiently reclaiming even a small portion of such waste heat would itself nearly satisfy the electricity needs of the planet [1]. Therefore, an attractive and sustainable solution to the energy problem would be the development of solid state thermal devices which could help recover this waste heat.

In an ideal model, a thermal rectifier is the thermal equivalent of the electrical diode. A device which conducts a greater heat flow in one direction than another one. Such thermal rectifiers could have huge impact as thermal energy harvesting devices, as well as heat control devices. Furthermore, in addition to heat control and harvesting; thermal diodes could be the basis for the development of more complex devices such as thermal transistors and even thermal logic devices [2,3]. There are currently two general approaches which can potentially result in rectifying behavior: bulk and molecular mechanisms. Bulk mechanisms basically include effects such as asymmetric electron transport at interface [4,5], strain-warping at interface between two solids [6–16], thermal potential barrier at interface [17–19], and temperature dependence of thermal conductivity at interface [20–30]. On the other hand, molecular mechanisms are based on non-uniform mass loading [31–35], asymmetric nanostructured geometry [36–56], nanostructured interfaces [57–60], anharmonic/nonlinear lattices [61–71], and quantum thermal systems [72–79]. In the experimental context, despite many decades of research, neither bulk nor molecular mechanisms have evidenced that the rectification factor can reach an order of magnitude, which is an arbitrary limit required to deem the effect useful for engineered systems, and the best reported rectification factors are 1.7 at 150 K [80] and 1.11 at 80 mK respectively [75], nevertheless, the low temperatures of operation make them unpractical. In the theoretical context, most suggestions based on nanoscale thermal rectification predict rectification factors ranging from 100 to 10000 [37,63,81,82], such systems require coupling and layout between individual atoms, which are

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very difficult to accomplish in practice. However, the only nanoscale thermal diode demonstrated at room temperature has shown a thermal rectification of 1.07 [31]. Clearly, much work remains to be done in order to achieve a practical, room temperature thermal rectifier with rectification factor up to theoretically predicted limits.

The basic idea of classical thermal rectification in a two segments device made of materials with opposite trends in their thermal conductivities $k(T)$ was initially proposed by Jesowski and Rafalowicz [22]. For these systems behave like thermal rectifiers, a clear difference in the temperature dependence of the thermal conductivity is necessary, as well as a large temperature gradients in order to induce thermal conductivity gradients along the device, as confirmed by C. Dames [29]. Furthermore, in such devices the rectification temperature (the *On-state* of the device) depends on the interface temperature which varies according to the thermal bias. As a result, the device lacks of a fixed forward temperature similar to the forward voltage in electronic diodes which controls accurately the “*on state*” of the device [83].

Heat transfer in solids basically depends on the electrical, magnetic and crystalline nature of materials via electrons, magnons and phonons respectively. Nevertheless, phonons play a major role in the thermophysical properties of condensed matter, such as specific heat and thermal conductivity. In this work, considering that a phonon is a collective vibration in a periodic, elastic arrangement of atoms or molecules; then, materials with single-stage solid–solid transformations can lead to thermal rectification via a change in the vibrational frequency of phonons in accordance with the promoted solid phase by the transition temperature. Unlike to former thermal diodes, the approach here presented can lead to thermal rectifiers with a well-defined *breakdown* as well as *forward bias temperatures* given by the exothermic transition temperature during forward and reverse bias mode respectively, which control accurately the *on state* of the device. This striking characteristic may open up important applications in thermal circuits and thermal management.

2. Experimental details

Fig. 1 shows a schematic view of the thermal diodes as well as the general experimental set up used during measurements. Basically, the device is formed by the junction of two material segments. One of the segments corresponds to Cu, Fe or graphite rod. Such materials were chosen because they present dissimilar acoustic properties. The other one segment is the material with the single-stage solid–solid transition [84], and in this case a Nitinol rod was chosen because it presents T_{endo} and T_{exo} which corresponds to the *martensite–austenite* and *austenite–martensite* transitions respectively [85–87]. Next, in order to ensure a good thermal contact between surfaces during heat transfer, a mirror finish was given to samples cross sections by using a standard metallographic polish technique, as well as by adding a highly thermal conductive thin layer of silver paste (Nanosilver Paste CK 4960 JET ART) onto surfaces. Finally, the thermal junctions were formed by bring together the surfaces of the Nitinol rod and the non-phase change material (Nitinol, Cu, Fe and Graphite segments were 2 mm length and 1.25 mm diameter).

In order to estimate the Nitinol exothermic T_{exo} and endothermic T_{endo} transition temperatures, DSC analysis was carried out using DSC-Q200 calorimeter by TA Instruments. The heating/cooling rate was performed in a range of 0 °C to 100 °C at a rate of 10 °C/min. Furthermore; to explore the thermal rectification effect under the AMM approach, a qualitative and quantitative investigation of the phase transition through the acoustic properties of a Nitinol, Fe, Cu and Graphite rods was carried out. Sound wave propagation was investigated when the materials are set to vibrate by an acoustic impulsive excitation focusing only convenient on the fundamental mode at selected T, say every 5 K from 285 to 385 K and backwards in a similar way as previously reported [88]. On the other hand, in order to obtain the acoustical impedance of the materials (the product of the sound velocity and mass density) it was necessary to measure the mass density by simply measuring the weight and the volume of each sample.

Q-ΔT *transfer characteristics* measurement system is basically as shown in Fig. 2. Thermal device is placed between heater element and Peltier element, and then silver paste is used to enhance thermal contact between diode and heater as well as cooler device. The heater and Peltier device are placed on Silica aerogel tiles (Shuttle tile insulator LI-900 from Kennedy Space Center) to reduce the heat leakage by conduction. Besides, the hot surface of Peltier device is air cooled via an air cooler. Two planar type K micro thermocouples are embedded just onto heater and Peltier surface to monitor the temperature rise between diode surfaces by using an external data acquisition card (National Instruments NI-9219).

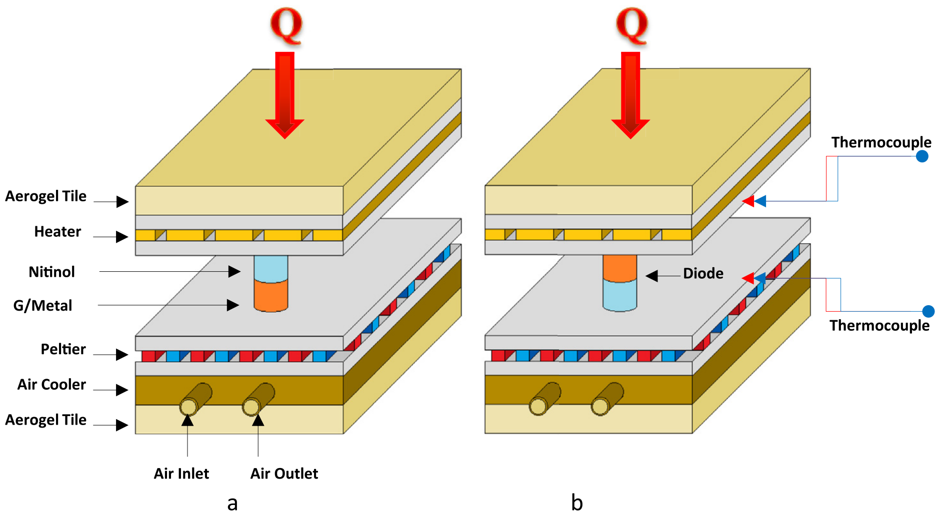

Fig. 1. Experimental set up. a) Reverse biased thermal diode and b) Forward biased thermal diode.