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► To cite this version:

Paul Desmarchelier, Efstratios Nikidis, Joseph Kioseoglou, Yoshiaki Nakamura, Anne Tanguy, et al.. Beyond Fourier Thermal Management at the Nanoscale. 28th International Workshop on Thermal Investigations of ICs and Systems, THERMINIC 2022, Sep 2022, Dublin, Ireland. 10.1109/THERMINIC57263.2022.9950603 . hal-04045463

HAL Id: hal-04045463

<https://hal.science/hal-04045463>

Submitted on 12 May 2023

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Beyond Fourier Thermal Management at the Nanoscale*

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Abstract—In this proceeding, we show diverse non Fourier effects that have been obtained with Molecular Dynamics simulations using silicon nanostructures and nanostructured materials. First, thermal rectification is observed in silicon nanowires with asymmetric amorphous shells. We then show that it is possible to design a pass band filter for phonons using a similar structure. Finally, phonon diffraction is obtained using two crystalline silicon blocks connected by silicon nanochannels.

Index Terms—Thermal Rectification, Phonon diffraction, Phonon filtering

I. INTRODUCTION

The understanding of the fundamental mechanisms of transport properties at the nanoscale enables the conceptualization and the elaboration of nanocomposites or nanostructured materials. These nanocomposites can be used for energy scavenging purposes [1], for thermal management purposes [2] or even information processing using phonons [3]. For example, interesting beyond-Fourier heat transport phenomena have been observed or proposed the last years as thermal rectification [4], phonon filtering [5], or phonons diffraction [6]. These beyond-diffusion phenomena could propose improvement of heat management at the nanoscale or even interesting new applications. For instance, the thermal rectification could enable the creation of smart materials that can dissipate or hinder heat depending on the ambient conditions, or the phonon diffraction could allow heat shielding to protect a device or on the contrary phonon focusing to create hot-spots. Phonon filtering on the other end may be useful in the field of phonon-based information process, which might be useful to select a frequency carrying information. While experimental set-ups

to observe beyond-Fourier behavior are still rather a difficult task, atomistic simulations have been applied with success. In this work, via Molecular Dynamics simulations, we will show that beyond-Fourier thermal properties can be achieved using amorphous/crystalline nanocomposites without requiring the use of complex crystalline structures. After a short methodology part, the results will show three cases in which non-diffusive behavior has been observed: thermal rectification for conical amorphous shell with crystalline core nanowires, phonon filtering for cylindrical core/shell nanowires and finally phonon diffraction patterns through a crystalline aperture.

II. METHODOLOGY

The Molecular Dynamics (MD) simulations are performed using the LAMMPS code [7]. The nanostructures of interest here are: crystalline silicon nanowires of constant diameter of 5 nm on which an amorphous shell (a-Si) is added (see Fig. 1 a and b). This amorphous shell is an approximation for the naturally occurring native oxide layers formed once silicon nanostructures are exposed to air [8]. The effect of the shape of this shell is studied by varying its shape, either using a constant thickness shell (a) or a varying thickness from left to right to obtain a conical shape (b). More information about the exact geometry can be found in [9]. The second configuration studied here is a block crystalline silicon, separated in two parts by a small crystalline channel as represented in Fig. 1-c. This block has periodic boundary conditions in all directions to reproduce an infinite transmission diffraction grating.

Two different approaches are used to appraise the thermal properties of the studied here nanomaterials using MD. The first one is a conventional method that allows computing an effective thermal conductivity: Non-Equilibrium Molecular

This work was granted access to the HPC resources of IDRIS under the allocation 2021-A0110911092, made by GENCI

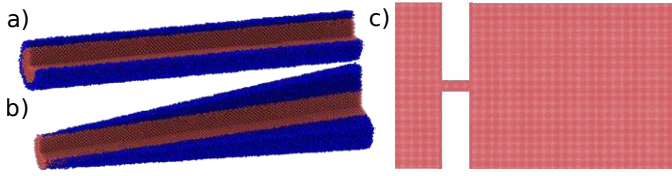


Fig. 1. Core-Shell Nanowires with a) a constant shell thickness or b) varying shell thickness and c) Crystalline silicon blocks separated by a crystalline channel. Crystalline silicon atoms are represented in red while amorphous silicon atoms in blue.

Dynamics (NEMD) [10]. This method is inspired by the hot/cold two plates experiment: a thermal gradient is created in the two extremities of the material by using two thermostats separated by a non thermostated region. Using the heat flux exchanged by the thermostats during the steady state and the temperature gradient through the structure, one can compute the thermal conductivity. A scheme of the configuration used here can be found in Fig. 2.



Fig. 2. Schematic representation of a NEMD simulation set-up with the hot region in red and the cold region in blue at the two extremities of the structure. To avoid distortion of the nanostructure some layers of fixed atoms are usually used after the thermostats. The extraction of the thermal properties concerns the distance L as depicted in the figure.

The second approach used here, it focuses directly on the vibrational properties and computes the Mean Free Path (MFP) of phonons using a wave-packet approach. The idea is to excite a narrow slice of atoms (in the center of the nanowire for instance) with a Gaussian windowed sinusoidal force excitation as represented in Fig. 3 to create a wave-packet at a given frequency and polarisation. The excitation is done at very low amplitudes on a system at mechanical equilibrium, this allows observing the effect of the nano-structuration on the wave-propagation. However, it does not take into account the effect of temperature, as we apply the wave at zero or very low temperatures with purpose to observe only the phenomena that we are willing, by avoiding the thermal noise. Then, from the wave-packet amplitude decay along the direction of propagation, the MFP can be computed using a fit to an exponential attenuation [9]. More broadly, this method can be used to study the frequency dependence of thermal properties, for instance to show diffraction and interference for specific frequencies in configurations such as the one presented in Fig. 1c.

III. RESULTS

A. Thermal Rectification

After calculating with the NEMD methodology the thermal conductivity of the conical tapered nanowires in both small

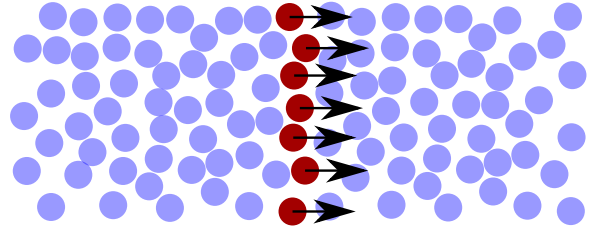


Fig. 3. Schematic representation of the layer of atoms being excited (in red). The arrows show the direction of the excitation.

to large and large to small diameter of nanowire directions, the rectification has been extracted and depicted in Fig. 4 as a function of the open angle of the conical shell. In a recent publications [9] we have shown that thermal rectification can be achieved. The rectification here relies on the asymmetry of the shell and appears for a conical shell with opening angles larger than 4.4° see Fig. 4. The rectification ($\eta = \frac{J_{SL} - J_{LS}}{J_{SL}}$) favors the transmission from the small cross section to the larger one. These results were obtained using NEMD simulations where the position of the thermostats have been inverted to compute the thermal conductivity in both directions (see Fig. 2). On the other hand, we have confirmed via Wave-Packet propagation simulations that the rectification is always observable and it may be caused by the interaction between the free surface and the amorphous crystalline interface creating direction dependent propagation [9]. As the effect is absent for lower opening angle it is very probably dependant on the thickness of the amorphous shell. The observed rectification coefficient is low but an optimization of geometries could enhance the phenomenon.

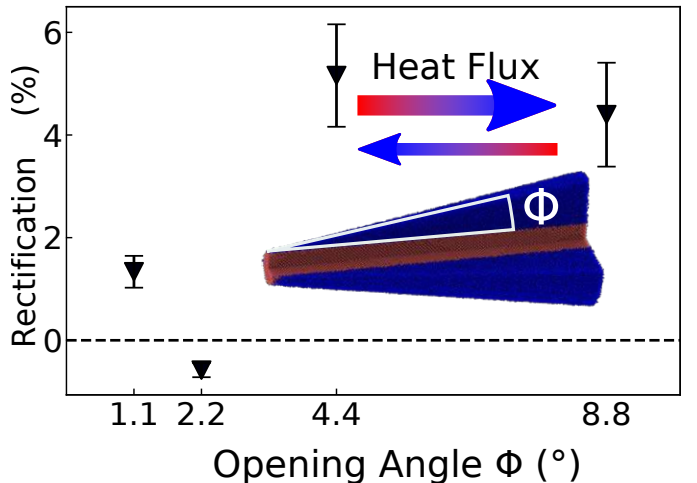


Fig. 4. Thermal rectification coefficient in percentage observed in conical core shell nanowires as a function of the conical amorphous shell opening angle. The heat flux is always stronger for the small to large nanowire cross-section. Silicon atoms in the crystalline phase are depicted in red (core), and in blue the atoms in the amorphous phase.

B. Phonon band-pass

Another interesting beyond-Fourier effect is the phonon band-pass, which can be observed in similar nanostructures; a crystalline core amorphous shell NW with constant diameter. It appears in Fig. 5 that a longitudinal excitation of frequencies around 10 THz has a much larger MFP (one order of magnitude higher) than the lower frequency phonons (2-4 THz). The drastic reduction of the MFP at low frequencies seems to be originated by the strong interaction between the crystalline core and the amorphous shell of the nanowire (see top inset of Fig. 5 – 3 THz), interaction that is not possible at higher frequencies where the wave-packets travels only through the crystalline core (see bottom inset of figure 1b -10 THz). Additionally, a kink in the slope at 7-8 THz can be observed in the figure 5. It corresponds to the end of the transverse acoustic phonon dispersion [11] (thus to a Van-Hove singularity) where more modes are available for scattering, decreasing the MFP.

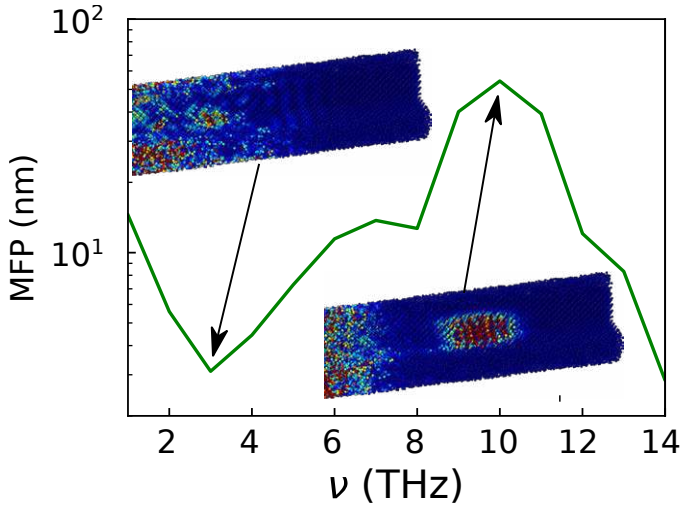


Fig. 5. Phonon Mean Free Path as a function of the excitation frequency for constant diameter crystalline-core amorphous-shell nanowires. The red/blue colors here corresponds to the kinetic energy associated with each atom: red is higher energy, blue is low one.

C. Phonon diffraction

The third beyond-Fourier effect studied here is the diffraction of high-frequency waves. For this, a wave-packet is generated in a left side of a Si crystal and then it encounters a barrier with an aperture. Here, the barrier is simply a void with a crystalline silicon channel as represent in Fig. 1c. The wave exiting the aperture experiences diffraction, as depicted in Fig. 6 at different time steps: as it exits the aperture (I), and as it spreads for two different time intervals (II-III). The observed patterns of the diffraction obtained with molecular dynamics simulations can be reproduced nicely using the Kirschhoff integral [12]. If the diffraction by a nanoconstriction has already been studied analytically [6], it is the first time to our knowledge that diffraction is shown using molecular dynamics simulations and for high frequencies waves (from 3 to 7 THz). This diffraction of high-frequency phonons

might be of importance for the design of thermal shields for electronic applications or other smart nanomaterials. A recent design of thermal shields has been proposed using a particle approach of phonon [5]. Here, we show that the wave nature of phonons must be considered at the small scale to adapt accordingly the design of heat management devices.

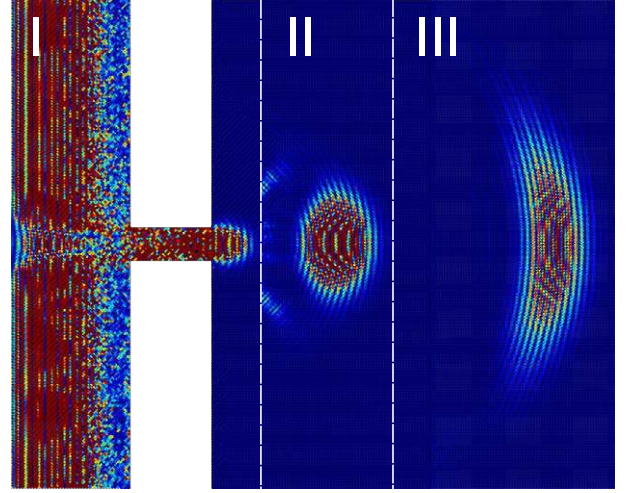


Fig. 6. Propagation of a plane wave transmitted through an aperture for three different times: just after reaching the aperture (I) and at two different time steps during the propagation, close and far from the aperture. The color scale represents the kinetic energy per atom as in the figure 5.

IV. CONCLUSION

Using simple nanostructures and nanocomposite materials (here crystalline and amorphous silicon), we show with atomistic simulations that it is possible to obtain exotic thermal phenomena beyond Fourier, which could be useful for thermal management. We show here that simple crystalline-core amorphous-shell nanowires can be used to obtain thermal rectification or to select phonon frequencies between 8 and 12 THz. Furthermore, phonon diffraction patterns could be obtained easily, showing that the wave-like nature of phonons should be considered for phonon focusing or thermal shielding applications. The non-Fourier thermal behavior observed here is caused by the combination of nanostructuration and/or combination of crystalline and amorphous phase.

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