Finite-element modeling of quasi-ballistic heat transport in nanostructured materials

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INTRODUCTION

Thanks to their ability to remarkably suppress phonon transport, nanostructured materials, such as nanoporous and nanocomposite materials, are recently gaining much interest for thermoelectric applications [1-3]. Molecular Dynamics (MD) simulations show that nanoporous Si can reduce the thermal conductivity up to two orders of magnitude with respect the bulk value [4]. However, to optimize thermal transport in such materials across a wide range of length scales, a continuous model is necessary. On the other hand, for materials whose characteristic length is smaller than the phonons mean free path, the Fourier's law breaks down and the ballistic heat transport becomes predominant. Here we present a Finite-Element (FE) approach to model quasi-ballistic heat transport and classical size effects by means of the Phonons Boltzmann Transport Equation (PBTE) under the relaxation time approximation. The model has been coded within the TiberCAD platform [5], which offers the key facilities for discretizing PDEs over a complex simulation domain. The developed module has been used for computing the phononic thermal conductivity (PTC) of porous Si composed by aligned squared pores. Pores size, spacing and surface roughness, have been varied in order to understand their effect on heat transport. Results, in agreement with those obtained by MD, provide an insightful guide for optimizing thermal transport from nano to macroscale.

RESULTS

The PBTE has been used to compute thermal transport across square-shaped aligned pores. Periodic boundary conditions have been applied to a unit cell composed of one pore whereas the heat flux is imposed to flow along the *x*-direction. The upper and lower boundaries are specular due to the symmetry and the pore walls are assumed diffuse (see Fig. 1). The PBTE has been spatially discretized by means of the Discontinuous Galerkin Methods [6]. For the sake of the simplicity, the medium has been assumed gray, *i.e.* physical properties such as phonons group velocity and scattering times are frequency-independent. The angular space has been discretized according to the Discrete Ordinate Methods (DOM). The thermal conductivity has been computed by varying the pore spacing, size and surface roughness. The temperature and flux maps are shown in Fig. 2. We found that the PTC can be lowered by decreasing the pore spacing because to the higher surface-to-volume ratio, which correlates with the classical size effects. Another way to decrease the PTC is increasing the pore size, which leads to higher porosity and, as a consequence, phonons have less volume in which they can travel (see Fig. 3). By varying the surface specular parameter we have found that the surface roughness plays an important role when the surface-to-volume ratio is higher (see Fig. 4), as expected. These results, in agreement with those obtained by MD simulations [4,7], reveal the suitability of the PBTE for addressing nanoscale thermal transport in nanoporous materials. Future developments may be devoted to the inclusion of the film thickness, which represents an additional reduction in the PTC [8]. Furthermore, by enlarging the unit cell, we will be able to include multiple pores in the calculation and hence investigate the correlation between pores disorder and PTC (see Fig. 5).

CONCLUSIONS

We have presented a PBTE based tool for computing thermal transport in nanostructured materials. As integrated in a FE element environment, the model can be solved for very complex geometries and coupled with electrical charge models, in order to simultaneously engineering the electrical and thermal transport of high-efficiency thermoelectric materials.

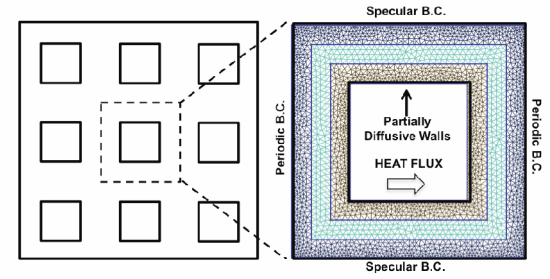

Fig. 1. (Left) Porous materials composed of aligned squared pores. (Right) Simulation domain and boundary conditions. Heat is enforced to flow from the left to the right side.

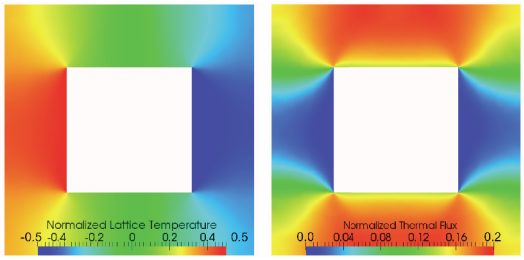

Fig. 2. (Left) Normalized temperature map. (Right) Magnitude of the normalized heat flux.

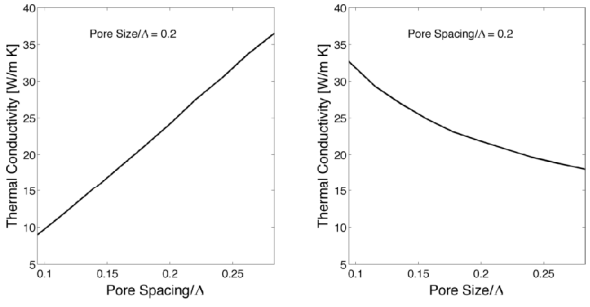

Fig. 3. Normalized thermal conductivity versus (left) pore spacing for a fixed pore size and (right) pore size for a fixed pore space.

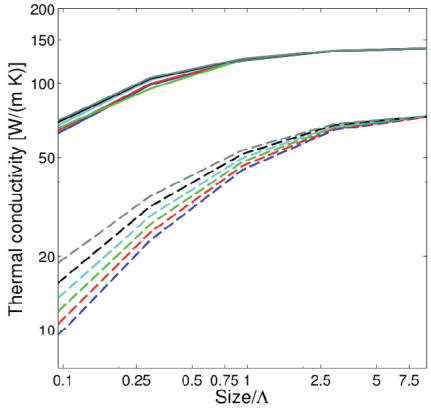

Fig. 4. Thermal conductivity versus the pore size for high and low porosity condition. The surface specular parameter *p* is varied from 0 to 1.

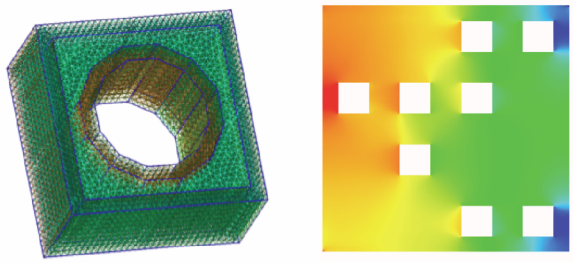

Fig. 5. (Left) Simulation domain of a thin film porous material. (Right) Normalized temperature map of a random pore configuration.

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