An Investigation of the Geometrical Effects on the Thermal Conductivity of Graphene Antidot Lattices

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Abstract

In this work we investigated the thermal conductivity of graphene-based antidots. The methods to reduce the thermal conductivity and improve the thermoelectric figure of merit of graphene based devices are studied. Our results indicate that triangular antidots have the smallest thermal conductivity due to longer boundaries and the smallest distance between nearest dots.

Introduction

The efficiency of thermoelectric devices for converting waste heat into useful electrical energy depends on the figure of merit $ZT=S^2\sigma T/(K_{el}+K_{ph})$, where S, σ, T, K_{el} and K_{ph} are the Seebeck coefficient, the electrical conductivity, absolute temperature, the electrical, and the lattice contributions to the thermal conductivity, respectively. Larger values of ZT indicate higher energy conversion efficiency.

Graphene, a recently discovered form of carbon that consists of only one layer of atoms arranged in a honeycomb lattice [1], has received much attention in the last few years for its intriguing electrical, optical and thermal properties. The electrical conductivity of the graphene sheet is higher than that of copper. A giant Seebeck coefficient has been reported for graphene [2]. These factors render graphene a candidate for future energy harvesting applications. However, the ability of graphene to conduct heat is an order of magnitude higher than that of copper [3]. Therefore, it is necessary to reduce its thermal conductivity. Recently, many studies have been conducted to investigate mechanisms that affect the thermal conductivity, such as the effects of boundaries [4], isotope doping [5] and defects [6].

Approach

In this paper we investigate the thermal conductivity of new graphene-based antidot lattice [7]. By introducing dots in the graphene sheet, see Fig.1, the transmission of phonons is significantly reduced which results in the reduction of the thermal conductivity. We represent the unit cell of the graphene antidot lattice by two parameters L and N, where L is the side length of the hexagon measured with the units of the graphene lattice constant a=2.46 Å and N is the number of carbon atoms that are removed from pristine super cell. We evaluate the phonon dispersion by using a 4th nearest-neighbor force constant method. Considering the phonon dispersion, one can find the ballistic phonon transmission from the density of modes.

Results

In Fig. 1(b), a circular antidot is shown. This antidot is created by removing 108 carbon atoms from the unit cell with L=10, therefore, represented by Circ(10,108). We considered dots with circular, rectangular, hexagonal, iso-triangular, and right-triangular shapes, see Fig. 1. For a fair comparison, we keep the area of different dots within 15%. Hence the number of carbon atoms that are removed from the pristine unit cell is nearly equal for different unit cells. The thermal conductivities of these structures are presented in Table 1. Although Circ(10,108), Hex(10,120), and Rect(10,120) have different areas, they have nearly the same circumference which results in nearly the same thermal conductivity. In addition, the distances between different dots in the corresponding lattices are equal. The areas of IsoTri(10,126) and RightTri(10,126) are 5% lower than those of Hex(10,120) and Rect(10,120), but their thermal conductivity is 30% smaller. This can be explained by two facts. First the circumferences of these dots are %25 larger than that of the Hex(10,120). Secondly, the distance between nearest dots in the corresponding two-dimensional lattice is smaller than in the Hex(10,120) lattice.

Conclusions

Our results indicate that not only the size of the dots, but also the circumference of the dots and distance between dots can strongly influence the thermal properties of graphene antidot lattices. We show that by appropriate selection of the geometrical parameters one can significantly reduce the thermal conductivity of graphene antidot lattices and improve their thermoelectric figure of merit.

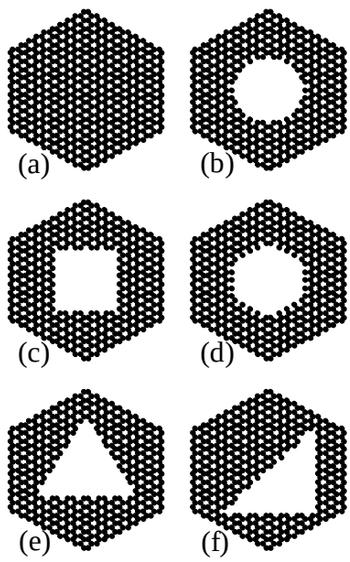

Fig. 1: Different antidot lattices which are studied in this work. (a)-(e) are the pristine graphene, Circ(10,108), Rect(10,120), Hex(10,120), IsoTri(10,126), and RightTri(10,126), respectively.

Table 1: Normalized thermal conductance of different antidots with respect to the pristine graphene.

Pristine Graphene	Circ (10,108)	Rect (10,120)	Hex (10,120)	IsoTri (10,126)	RightTri (10,126)
1	0.2694	0.2462	0.2696	0.1916	0.1834

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