Thermal Properties of Graphene Antidots

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Disorder and roughness can effectively reduce the thermal conductivity and enhance the thermoelectric properties of the material. In this work we study the effect of periodic holes (antidot lattice) on the thermal conductivity of graphene. Our results indicate that by increasing the radius of the dot the phonon density of states decreases dramatically, resulting in the improvement of thermoelectric properties of graphene.

Graphene, a recently discovered form of carbon (1), has received much attention over the past few years, due to its excellent electrical, optical, and thermal properties. A giant seebeck coefficient has been reported for graphene (2). However, to apply graphene for thermoelectric applications it is necessary to reduce its thermal conductivity. Recent studies show that boundaries and edge roughness have strong effects on the thermal conductivity (3). Here we investigate the thermal properties of a new graphene-based structure, which is called graphene antidote lattice (4). As these structures have many boundaries, see Fig. 1(a), one should expect a very low thermal conductivity in comparison with pristine graphene. The unit cell of a graphene based antidot is described with the parameters (L,R), where L and R are the side length of the hexagonal unit cell and the radius of the hole, respectively. Both L and are measured with the units of the graphene lattice constant $a = 2.46$ Å. We calculated the phonon dispersion and density of state (DOS) using the force constant method including 4th nearest neighbors. Fig.1(b) shows the DOS of antidots with L=10 and different radiuses. As shown in Fig. 1(b), by increasing R the phonon DOS and the thermal conductivity are significantly reduced. As a result, thermoelectric properties are improved.
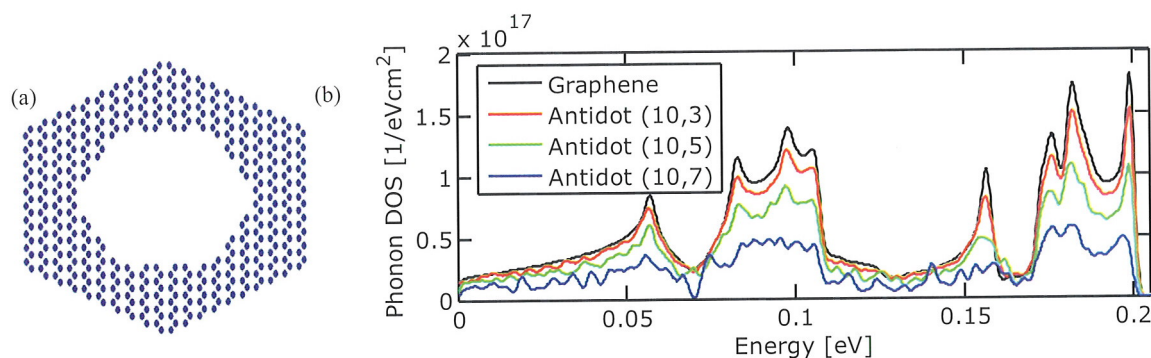

Fig.1: (a) Unit cell of a (10,5) antidot. (b) Phonon DOS of pristine graphene and antidots with L=10 and R=3,5,7.

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