Finite Element Method (FEM) Simulation on Snowflake Shaped Graphene Phononic Crystal

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Phonons are collective mechanical lattice vibrations that are responsible for transmission of sound (low frequency oscillation of mechanical waves in KHz regime) and heat (high frequency oscillation of mechanical waves in THz regime) through materials. Phonon engineering involves the control of heat transport in materials by introducing artificial phonon structures which reduce the thermal conductivity either by the particle model (utilizing phonon scattering at the surface/interface of materials) or the wave nature model (suppressing the propagation of phonons via phonon confinement induced by lattice periodicity). Recent studies on the control and manipulation of thermal phonons show that specifically designed periodic arrays can reduce the thermal transport through a material by suppressing the transmission of a certain phonon wavelength [1,2]. We have developed a technique to fabricate suspended graphene phononic crystal (GnPC) with 3-4 nm pore size and sub-10-nanometer pitch using the helium ion beam milling (HIM) technique [3]. Subsequently, it has been observed by FEM simulations considering longitudinal phonon vibration that, in case of graphene, periodic nanopores with sub-10 nm pitch exhibit phononic band gap (PnBG) in the low THz regime [4]. To explore the possibilities of PnBG generation in higher THz regime in GnPCs, we were motivated to proceed with three dimensional FEM studies for more complex pore shapes and variable pore sizes.

It has been reported that the confinement of phonon modes in the narrow constrictions of the cross shaped structures provide a favorable condition for PnBG generation [5]. Now the study has been extended for the hexagonal lattice counterpart (called a snowflake structure) of the cross substrate as shown in fig-1(a). The study has been carried out on the minimum unit cell (fig-1(b)) with periodic boundary conditions. Considering graphene with the thickness of 1nm to favor the meshing condition in COMSOL multiphysics software, we observed the PnBG opening for snowflake structures with different pitch and neck length. To keep consistency with our previous study with the cross shaped pores, the porosity was kept ~ 0.28 for this study as well. We have observed that, for the same porosity and pitch, the PnBG appears with parallel dispersion branches at higher frequency regime (~1.6 THz) in the snowflake structure compared to that of the cross structure (~0.9 THz) [5] as shown in the phonon dispersion curve in fig. 2. Also, decreasing the pitch size results in the phonon dispersion to shift to higher frequencies. A complete bandgap map is shown in fig.3 for the structure with varied neck width(w)/pitch(p) ratio where the most prominent bandgaps are generated at w/p = 3.8 and w/p = 2.7. In the meeting, further studies demonstrating the PnBG dependence on various phonon modes will be discussed to clarify the origin of PnBG.

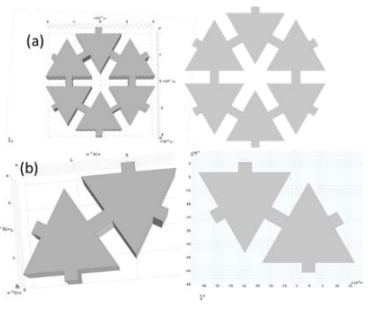

Fig 1 *(a) Simulation model of GnPC with snowflake shaped nanopore. (b) Actual model reduced to minimum unit cell with periodic boundary condition.*

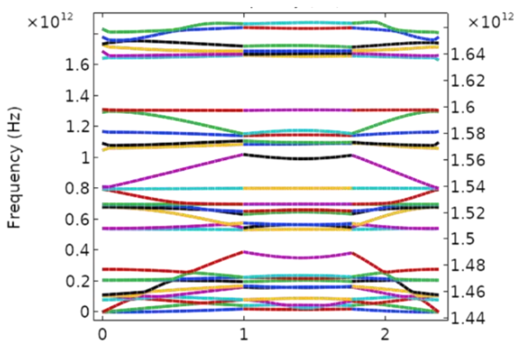

Fig 2 *Phonon dispersion curve for snowflake shaped GnPC with 25 nm pitch and 0.28 porosity.*

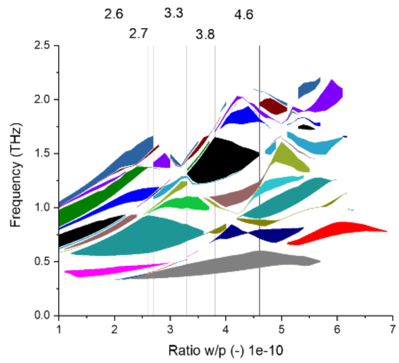

Fig 3 *Complete phononic bandgap map for snowflake shaped GnPC for different w/p ratio.*

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