THEORETICAL CALCULATION OF THIRD ORDER SUSCEPTIBILITY OF ARMCHAIR GRAPHENE NANORIBBON AT NEAR INFRARED RANGE

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Since the isolating of graphene, the single layer of carbon atoms in 2D honeycomb structure, much research efforts has been expended to clarify the electronic and optical properties, and to apply them to novel electronic and optoelectronic devices. Most of optoelectronic devises made by graphene nanoribbons, because of the energy gap in their band structure [1]. In this paper we report third order susceptibility of armchair graphene nanoribbons at near infrared (NIR) frequencies. The Calculation results show that Armchair graphene nanoribbon has high nonlinear response, as the third order susceptibility has the order of 10-7(esu).
To calculate the nonlinear effects, first we have calculated the band structure and band gap energy of Armchair garphenen nanoribbon (A-GNR) by including the edge deformation (the edge carbon atoms of A-GNR are all passived by hydrogen atoms) with Tight-binding model [2]. There are three distinct families for A-GNRs: N=3m, N=3m+1 and N=3m+2, with integer m, where N indicates the number of unit cells across the ribbon width.
Figure 1 shows the energy gaps of three families of A-GNRs for different widths of ribbon. As depicted in the figure, with increasing the ribbon widths, the band gap energies are decreasing. However to detuning the band gap energy of the system for optical applications, we should optimize the shape and the width of graphene nanoribbon.
Knowing the band structures, we used Genkin-Mednis approach [3] to calculate the third order susceptibility. In which allows us to determine $\chi^{(3)}$ in two band approximation, where the main contribution to $\chi^{(3)}$ is determined by the highest valence band (v-band) and lowest conduction band (c-band). For A-GNRs without doping, while a part of the bands is completely filled whereas the remaining ones are empty, we consider only the interband transition for estimating the interband third order susceptibility of A-GNRs. In one electron approximation and by using Genkin-Mednis, one can calculate total polarization and third order polarization of system, and then obtain interband third order susceptibility in two band approximation. For this purpose we consider that all the electromagnetic fields are polarized along the nanoribbon axis. In this case the component χ_{yyyy}=$\chi^{(3)}$ of the third-order nonlinear optical susceptibility tensor $\chi^{(3)}_{\mu\alpha\beta\gamma}(\Omega, \omega_1, \omega_2, \omega_3)$ are considerable [4]. For calculating the matrix element of an interband transition we follow Gupta et al. [5], that obtained matrix elements for high-order harmonics of graphene.
We have used generation of mixed optical frequency harmonics $2\omega_1 - \omega_2$ under irradiation of two monochromatic waves with the frequencies $\omega_1 = 0$ and $\omega_2 = \omega$. Results are shown in

figures 2 and 3. Fig. 2 shows the dependence of imaginary part of $\chi^{(3)}$ to width of nanoribbon for two families of A-GNR. This figure shows that N=3m+1 family, with wider band gap in comparison with other family, has lower $\mathrm{Im}(\chi^{(3)})$. Also, Interband third order susceptibility increase by increasing the width of nanoribbon (decreasing the energy gap).
Figure 3 shows the real and imaginary parts of Interband third order susceptibility, for different width of A-GNR, in which have plotted at near infrared energy rang. This figure shows that there is high nonlinear optical susceptibility for A-GNRs in NIR range, from order of $\sim 10^{-7}$(esu), which is 10^8 times higher than insulating materials ($\sim 10^{-15}$(esu)) [6]. This considerable difference between the nonlinear response of A-GNRs and insulating materials is due to the interband transitions in A-GNR and resonance in gap energies.

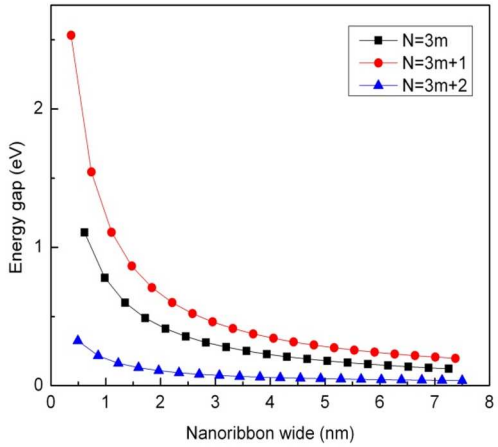

Figure 1: Energy gap of A-GNR for different three families by including the edge deformation (edge atoms passivated by hydrogen).

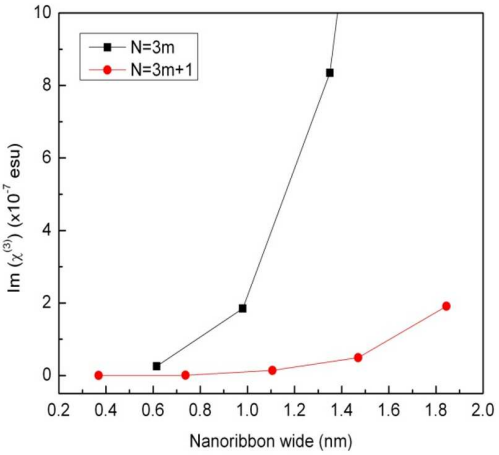

Figure 2: Imaginary part of third order susceptibility for A-GNR with different wide.

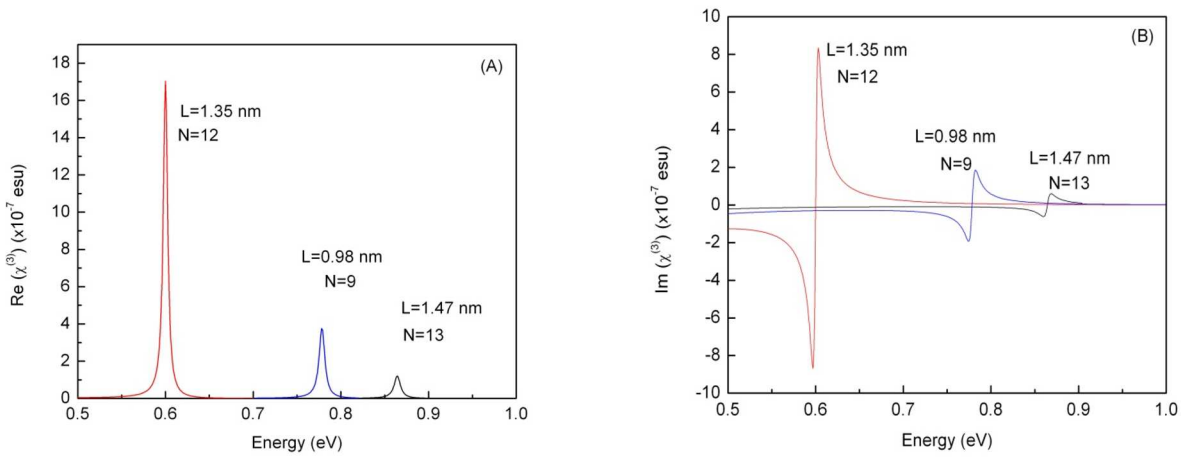

Figure 3: Real (A) and imaginary part (B) of interband third order susceptibility ($\chi^{(3)}$) for A-GNR with different widths (L) in NIR energy range. N indicates the number of unit cells across the garphene nanoribbon.

References

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