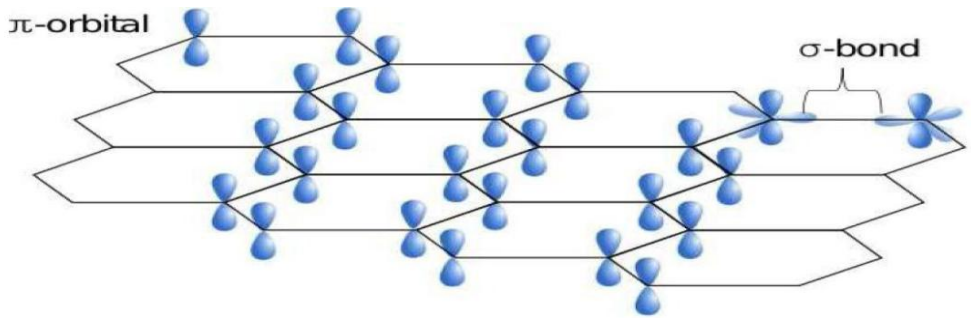
Thermoelectric Properties of Graphene and its applications

Dr S R Chaudhari
Department of physics, Research Center,
P.D.E.A's Baburaoji gholap college,sangvi,pune 27

Abstract : Grapheme has many applications Several fundamental questions on phonon scattering mechanism remains unanswered, which motivates us to carry out a systematic theoretical investigation of thermal and electrical properties of graphene using phonon scattering mechanism In present work we plan to develop the theoretical models for investigation of Two-dimensional lattice thermal transport, electrical conductivity, Seebeck coefficient, Specific Heat and thermoelectric figure of merit in graphene using phonon scattering mechanism. In proposed work we plan to incorporate the scattering of phonons with defects, grain boundaries, electrons, out-of-plane phonon and umklapp phonon scatterings in the model Hamiltonian within the relaxation time approximation to demonstrate the anomalies observed in thermal conductivity of graphene. It seems that the thermoelectric properties can be well explained using the Debye like model based on phonon scattering mechanism. Results drawn from proposed work are expected to useful in designing the future applications based on graphene

Introduction : Graphene physically acts as a 2-Dimensional material. This leads to many properties that are electrially beneficial, such as high electron moblity and lowered power usage. Graphene is currently in its infant stages and is undergoing many applications and studiesGraphene is a 2-dimensional honeycomb lattice of carbon atoms:



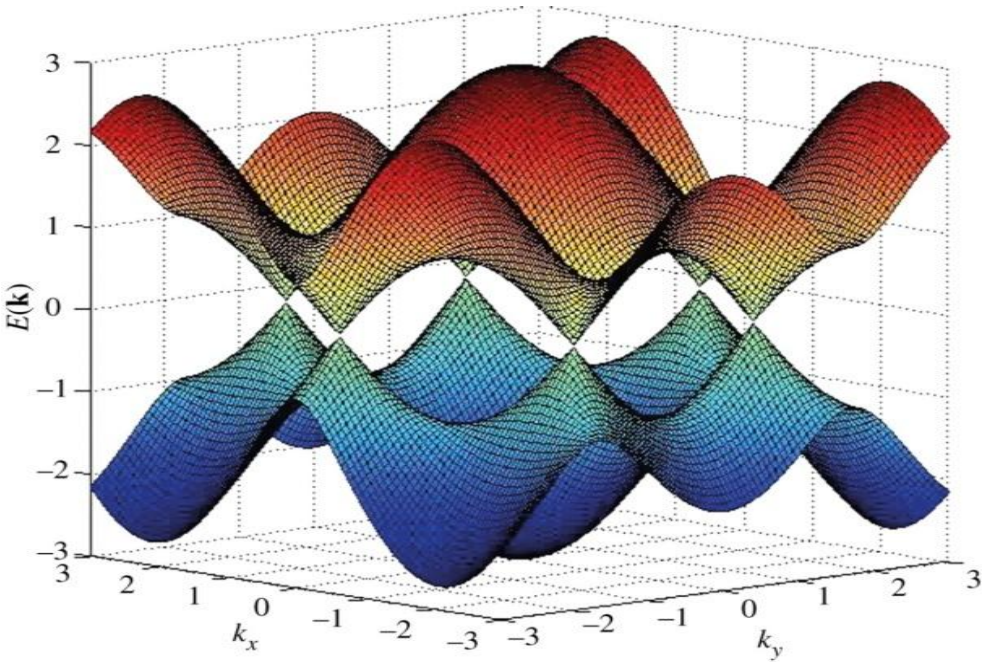
Each carbon atom has 3 valent electrons. 3 of them form chemical bonds between atoms (σ-orbitals), another one forms π-orbital (sp3 – hybridization

Theory :Properties of Graphene :electronic properties

There can only be a maximum of two electrons on the π-orbital. Graphen at «half-filling» (zero chemical potential): the number of electrons on π-orbitals is equal to the number of atoms.

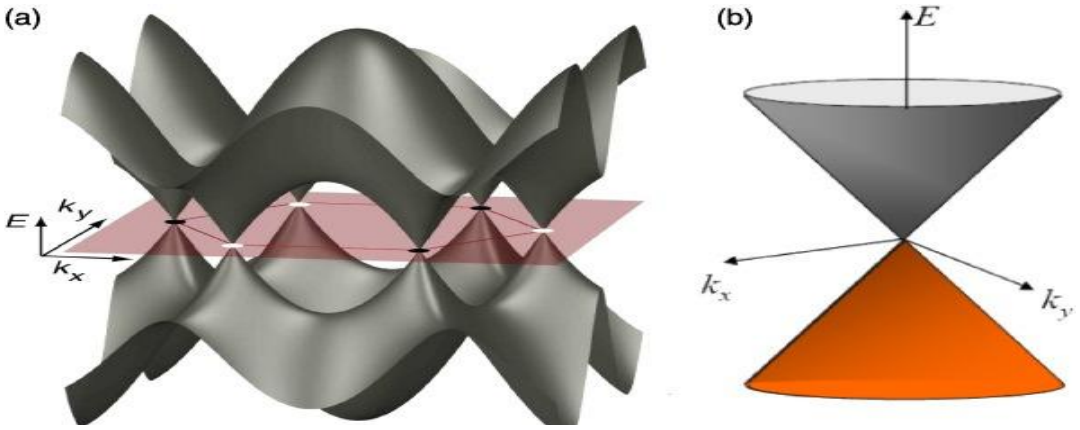
Therefore, electrons on π-orbitals can easily move from one atom to the neighbouring one thus determine the electronic properties of graphene.

Dispersion relation:



Dirac cones appear at the 2 non-equivalent points within the Brillouine zone. So, low-energy excitations can be described as 2 flavours of 4-component massless Dirac fermions. Graphene is a semi-metal: Fermi surface is reduced to the «Fermi-points»

Electronic Structure:Dirac Points are the transition between the valence band and the conduction band.The six Dirac points can be divided into to two in-equivalent sets of three (K and K'), represented by the black and white dots on part (a) The points within each set are all equivalent because they can reach each other by reciprocal lattice vectors Part (b) shows that the dispersion relation close to the K points looks like the energy spectrum of massless Dirac particles .



2) Electrical Properties:The Fermi level can be changed by doping to create a material that is better at conducting electricity.Experimental graphene's electron mobility is 15,000 cm2/(V*s) and theoretically potential limits of 200,000 cm2/(V*s) Graphene electrons are like photons in mobility due to lack of effective electron and hole mass.These charge carriers are able to travel sub-micrometer distances without scattering .

Table I Values of electron mobility and energy bandgap for Hall effect sensor materials

	$\mu(cm^2\ V^{-1}\ s^{-1})$	E_g (eV)
Silicon	1,900	1.12
GaAs	8,800	1.43
InSb	78,000	0.17
InAs	33,000	0.35
InP	4,800-6,800	1.29
2-DEG	6,500-13,000	0.6-1.8

3) Mechanical Strengths:Bond length is .142 nm long = very strong bond Strongest material ever discovered ultimate tensile strength of 130 gigapascals compared to 400 megapascals for structural steel Very light at 0.77 milligrams per square metre, paper is 1000 times heavier Single sheet of graphene can cover a whole football field while weighing under 1 gram Also, graphene is very flexible, yet brittle .

4) Optical PropertiesAbsorbs 2.3% white light Optical electronics absorb <10% white light Highly conductive Strong and flexible

Methodology :Graphene that consists of only one plain layer of carbon atoms arranged in a honeycomb lattice [1] has attracted tremendous interest for both fundamental studies and applications in high-speed electronic devices because of its extremely high carrier mobility [2-4], outstanding

thermal transport property [5-8] and Seebeck coefficient [9]. The extremity high observed thermal conductivity (κ) [5-8] of graphene establishes it as an excellent material for thermal management. With the continuously decreasing size of electronic devices and increasing dissipation power density in downscaled circuits, one observes a tremendous growth of materials that can conduct heat efficiently. Besides carbon nanotubes (CNTs) those are known to have very high thermal conductivity κ with the experimentally determined room temperature value of thermal conductivity ranging from ≈ 1500 to 6000 Wm-1K-1 for different structures of CNTs [10-12], the single plane layer of carbon atoms (i.e. graphene) are another structures who demonstrates an extremely high thermal conductivity.

Scattering by in-plane phonons

$$\varrho_{in} \approx \frac{8\hbar k_F^2}{e^2 \rho v_F^2 k_B T} \sum_{\nu} \int_0^1 dx \, [D_B^{\nu}(2x)]^2 \frac{x^4}{\sqrt{1-x^2}} \frac{e^{xz_\nu}}{(e^{xz_\nu}-1)^2},$$

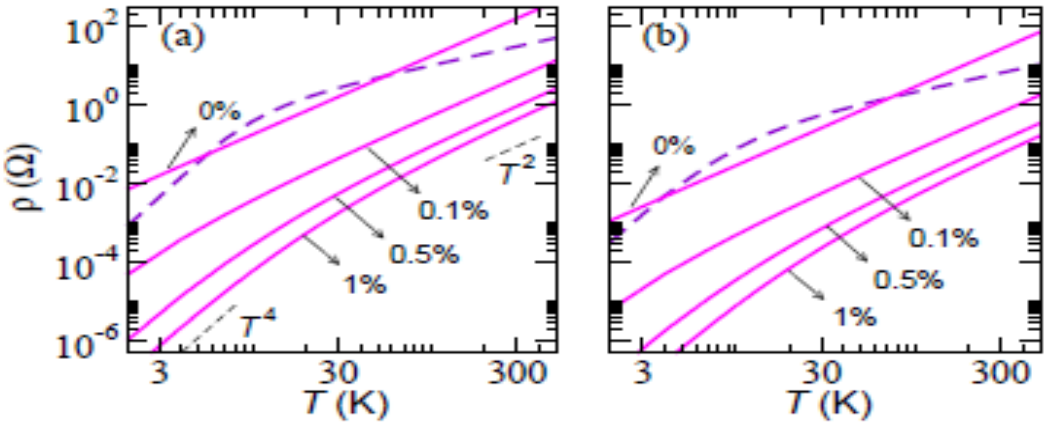


Figure 2: Resistivity vs T due to scattering by in-plane phonons (dashed thick lines) and flexural phonons (full lines) with and without strain (indicated in percentage), in monolayer (a) and bilayer graphene (b). We use $n = 10^{12}\,\mathrm{cm}^{-2}$, $g \approx 3\,\mathrm{eV}$, and $\beta \approx 3$.

Result and conclusion

- Graphene is also a potential candidate for application in thermoelectric energy conversion [13], where low κ but high electric conductivity (σ) for is required for obtaining high thermoelectric efficiency.
- To achieve high ZT for graphene, a general scheme is to minimize κ while keeping σ and Seebeck coefficient (S) less changed.
- One possible method is to dope the graphene with the stable isotope C13 since electronic structure of graphene is unchanged in this doping.
- In a pure crystal, one without defects or dislocations, phonon scattering in the presence of different isotopes has been strongly correlated with changes in thermal conductivity.
- It is observed that the κ of graphene is significantly reduced by ∼80%, in both armchair and zigzag directions, when a random distribution of C12 and C13 is assumed at different doping concentrations [14].
- The various experimental observations and theoretical reports emphasis that the propagation of phonons in an ordered single plane layer of carbon atoms, play an important role in the heat transmission in the graphene and responsible for high observed thermoelectric properties.
- Despite of several investigations the exact role of phonons, the phonon scattering mechanism in graphene, the phonon relaxation rates, dependence of phonon relaxation rates on temperatures and frequency and their effect on thermal conductivity is not clearly understood.

Future scope:. In proposed work we plan to incorporate the scattering of phonons with defects, grain boundaries, electrons, out-of-plane phonon and umklapp phonon scatterings in the model Hamiltonian within the relaxation time approximation to demonstrate the anomalies observed in thermal conductivity of graphene. It seems that the thermoelectric properties can be well explained using the Debye like model based on phonon scattering mechanism. Results drawn from proposed work are expected to useful in designing the future applications based on graphene

References

[1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva and A. A. Firsov, Electric Field Effect in Atomically Thin Carbon Films, Science 306 (2004) 666-669.

[2] Y. Zhang, Y. Tan, H. Stormer and P. Kim, Experimental observation of the quantum Hall effect and Berry's phase in graphene, Nature 438 (2005) 201-204.

[3] K. Wakabayashi, Y. Takane and M. Sigrist, Perfectly Conducting Channel and Universality Crossover in Disordered Graphene Nanoribbons, Phys. Rev. Lett. 99 (2007) 036601-4.

[4] A. H. Castro Neto, F. Guinea, N. M. Peres, K. S. Novoselov and A. K. Geim, The electronic properties of graphene, Rev. Mod. Phys. 81 (2009) 109-162.

[5] Michael Thompson Pettes, Insun Jo, Zhen Yao and Li Shi, Influence of Polymeric Residue on the Thermal Conductivity of Suspended Bilayer Graphene, 2011 Nano Lett. 11 1195–1200.

[6] A. A. Balandin, S. Ghosh, W. Bao, I. Calizo, D. Teweldebrhan, F. Miao, and C. N. Lau, Superior Thermal Conductivity of Single-Layer Graphene, Nano Lett., 8, (2008) 902-907.

[7] A. A. Balandin, Thermal properties of graphene and nanostructured carbon materials, Nature Mater. 10 (2011) 569-581.

[8] K. K. Choudhary, Investigation of two-dimensional lattice thermal transport in bilayer graphene using phonon scattering mechanism, Physica E 58 (2014) 106–110.