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A PROPERTIES OF GRAPHENE

Tarun M Radadiya

Student, Electronics and Communication Department, Gujarat Technological University (GTU), Vadodara, Gujarat India.

ABSTRACT: Graphene is pure carbon in the form of a very thin, nearly transparent sheet, one atom thick. It is remarkably strong for its very low weight (100 times stronger than steel and it conducts heat and electricity with great efficiency. Graphene with the unique combination of bonded carbon atom structures with its myriad and complex physical properties is poised to have a big impact on the future of material sciences, electronics and nanotechnology. Owing to their specialized structures and minute diameter, it can be utilized as a sensor device, semiconductor, or for components of integrated circuits. The reported properties and applications of this two-dimensional form of carbon structure have opened up new opportunities for the future devices and systems.

KEYWORDS: Graphene, Carbon, Atom, Electricity, Nanotechnology, Semiconductor, Integrated Circuits

INTRODUCTION

Graphene is a crystalline allotrope of carbon with 2-dimensional properties. In graphene, carbon atoms are densely packed in a regular sp^2 -bonded atomic-scale chicken wire (hexagonal) pattern. Graphene can be described as a one-atom thick layer of graphite. It is the basic structural element of other allotropes, including graphite, charcoal, carbon nanotubes and fullerenes. It can also be considered as an indefinitely large aromatic molecule, the limiting case of the family of flat polycyclic aromatic hydrocarbons.

Graphene research has expanded quickly since the substance was first isolated in 2004. Research was informed by theoretical descriptions of graphene's composition, structure and properties, which had all been calculated decades earlier. High-quality graphene also proved to be surprisingly easy to isolate, making more research possible.



Snapshot 5

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Snapshot 6

Andre Geim and Konstantin Novoselov at the University of Manchester won the Nobel Prize in Physics in 2010 "for groundbreaking experiments regarding the two-dimensional material graphene".^[4]

The global market for graphene is reported to have reached \$9 million by 2014 with most of these sales being concentrated in the semiconductor, electronics, battery energy and composites. However, the market is set to rapidly grow to ~\$100 billion as the material makes further inroads into the silicon market for highly integrated circuits and also in boosting the performance of lithium batteries.



Figure 1: Idealized structure of a single graphene sheet.

Chemical Properties

Graphene is the only form of carbon (and generally all solid materials) in which each single atom is in exposure for chemical reaction from two sides (due to the 2D structure). It is known that carbon atoms at the edge of graphene sheets have special chemical reactivity, and graphene has the highest ratio of edgy carbons (in comparison with similar materials such as carbon nanotubes). In addition, various types of defects within the sheet, which are very common, increase the chemical reactivity.

Mechanical Properties

Another of graphene's stand-out properties is its inherent strength. Due to the strength of its 0.142 Nm-long carbon bonds, graphene is the strongest material ever discovered, with an ultimate tensile strength of 130,000,000,000 Pascals (or 130 gigapascals), compared to 400,000,000 for A36 structural steel, or 375,700,000 for Aramid (Kevlar). Not only is graphene

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extraordinarily strong, it is also very light at 0.77milligrams per square metre (for comparison purposes, 1 square metre of paper is roughly 1000 times heavier). It is often said that a single sheet of graphene (being only 1 atom thick), sufficient in size enough to cover a whole football field, would weigh under 1 single gram.

What makes this particularly special is that graphene also contains elastic properties, being able to retain its initial size after strain. In 2007, Atomic force microscopic (AFM) tests were carried out on graphene sheets that were suspended over silicone dioxide cavities. These tests showed that graphene sheets (with thicknesses of between 2 and 8 Nm) had spring constants in the region of 1-5 N/m and a Young's modulus (different to that of three-dimensional graphite) of 0.5 TPa. Again, these superlative figures are based on theoretical prospects using graphene that is unflawed containing no imperfections whatsoever and currently very expensive and difficult to artificially reproduce, though production techniques are steadily improving, ultimately reducing costs and complexity.

The onset temperature of reaction between the basal plane of single-layer graphene and oxygen gas is below 260 °C [[]and the graphene burns at very low temperature (e.g., 350 °C). It should be considered that this specious interlayer is mostly due to the graphene curvature rather than to filling with functional groups (as in the case of graphite oxide). Owing to the high accessibility and active sites over a large surface area, this graphene sample shows a superior electrochemical behavior for hydrogen storage.

The importance of an edge to a graphene sheet parallels that of a surface to a crystal. Cutting through an infinite graphene sheet [Fig. 2(a)], one first breaks C-C s bonds and then obtains two semi-infinite graphene sheets, each with a one-dimensional edge. The dangling s bonds at the edges can be saturated with hydrogen (so-called hydrogenated or hydrogen-terminated edges) and all the carbon atoms remain sp2 hybridized. Depending on the cutting direction, two unique types of edges can be obtained: zigzag [Fig. 2(b)] and armchair [Fig. 2(c)]. The cutting also introduces a boundary at the edge to the previously fully delocalized p-electron system. It turns out that the geometry of the edge makes a huge difference in the p-electron structure at the edge. By constructing an analytical solution to the edge state, Nakada etval.3 showed that the zigzag edge in a semi-infinite graphene sheet gives rise to a degenerate flat band near the Fermi level for the k vector between $2\pi/3$ and p. For k= π , the wavefunction is completely localized at the edge sites, leading to a so-called localized state at the zigzag edge.

This flat-band feature and its corresponding localized state are unique to the zigzag edge (they are completely absent from the armchair edge).

Flexibility, mechanical properties of graphene fibers.

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Figure 3 (a) the end of the twisted fiber



Figure 3 (b) the middle of the twisted fiber







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(b)



(c)

Figure 2: Cutting through an infinite graphene sheet (a) to obtain a semi-infinite sheet with a hydrogenterminated zigzag (b) or armchair (c) Edge.

Electronics Properties

Graphene is a semi-metal or zero-gap semiconductor. Four electronic properties separate it from other condensed matter systems. One of the most useful properties of graphene is that it is a zero-overlap semimetal (with both holes and electrons as charge carriers) with very high electrical conductivity.



Figure 3 (d) Typical strain-stress curves of the single GO and graphene fiber. The inset photograph showing the testing state of the single fiber.

Mechanical properties of graphene-coated aerogels

Lightweight materials that are both highly compressible and resilient under large cyclic strains can be used in a variety of applicationsCarbon nanotubes offer a combination of elasticity, mechanical resilience and low density, and these properties have been exploited in nanotube-based foams and aerogels. However, all nanotube-based foams and aerogels developed so far undergo structural collapse or significant plastic deformation with a reduction in compressive strength when they are subjected to cyclic strain. Here, we show that an inelastic aerogel made of single-walled carbon nanotubes can be transformed into a superelastic material by coating it with between one and five layers of graphene nanoplates. The graphene-coated aerogel exhibits no change in mechanical properties after more than 1×10^6 compressive cycles, and its original shape can be recovered quickly after compression release. Moreover, the coating does not affect the structural integrity of the nanotubes or the compressibility and porosity of the nanotube network. The coating also increases Young's modulus and energy storage modulus by a.

Carbon atoms have a total of 6 electrons; 2 in the inner shell and 4 in the outer shell. The 4 outer shell electrons in an individual carbon atom are available for chemical bonding, but in graphene, each atom is connected to 3 other carbon atoms on the two dimensional plane, leaving 1 electron freely available in the third dimension for electronic conduction. These highly-mobile electrons are called pi (π) electrons and are located above and below the graphene sheet. These pi orbitals overlap and help to enhance the carbon to carbon bonds in graphene. Fundamentally, the electronic properties of graphene are dictated by the bonding and anti-bonding (the valance and conduction bands) of these pi orbitals.

Tests have shown that the electronic mobility of graphene is very high, with previously reported results above $15,000 \text{ cm}_2 \cdot \text{V}_{-1} \cdot \text{s}_{-1}$ and theoretically potential limits of $200,000 \text{ cm}_2 \cdot \text{V}_{-1} \cdot \text{s}_{-1}$ (limited by the scattering of graphene's acoustic photons). It is said that graphene electrons act very much like photons in their mobility due to their lack of mass. These charge carriers are able to travel sub-micrometer distances without scattering; a phenomenon known as ballistic transport. However, the quality of the graphene and the substrate that is used will be the limiting factors. With silicon dioxide as the substrate, for example, mobility is potentially limited to $40,000 \text{ cm}_2 \cdot \text{V}_{-1} \cdot \text{s}_{-1}$.

Graphene Brillouin Zone and Electronic Energy Dispersion

Graphene is a single layer of carbon atoms densely packed in a honeycomb lattice. The energy structure of crystals depends on the interactions between orbitals in the lattice. The tight binding approximation (TB) neglects interactions between atoms separated by large distances—an approximation that greatly simplifies the analysis.

Factor of ~ 6 , and the loss modulus by a factor of ~ 3 . We attribute the superelasticity and complete fatigue resistance to the graphene coating strengthening the existing crosslinking points or 'nodes' in the aerogel.

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Figure 4 (a) nanotube aerogels collapse and graphene-coated aerogels recover their original shape after compression by ≥90% (Supplementary Movie S1).



Figure 4 (b), σ versus ε curves for nanotube aerogels along the loading direction and for graphene-coated aerogels during loading–unloading cycles.

solid-state physics, the TB mode calculates the electronic band structure using an approximate Set of This Demonstration calculates and plots the tight-binding (TB) electronic band structure of graphene as the 2D hexagonal carbon crystal. The band structure of graphene is obtained from the TB approximation including only first-nearest-neighbor carbon-carbon interactions of π -orbitals of a single honeycomb graphite sheet. This is given by a simple analytical relation, derived by diagonalization of the 2×2 Bloch Hamiltonian for the diatomic graphene unit cell.

$$E_{v,c}(k_x, k_y) = \frac{\epsilon \pm t \, w(k_x, k_y)}{1 \pm s \, w(k_x, k_y)} \quad \text{with } (+) \Rightarrow v, (-) \Rightarrow c$$
$$w(k_x, k_y) = \sqrt{1 + 4 \cos\left(\frac{\sqrt{3} k_x \, a}{2}\right) \cos\left(\frac{k_y \, a}{2}\right) + 4 \cos^2\left(\frac{k_y \, a}{2}\right)}$$
with the phase factor

with the phase factor

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In this expression, *t* is the TB hopping parameter (overlap integral between π -orbitals), *t* is the on-site energy parameter, *t* is the overlap parameter, *a* is the lattice parameter of graphene, the vand *c* indices stand for valence and conduction bands, respectively, and $k = (k_x, k_y)$ represents the 2D wavevector components along the *x* and *y* directions in the 2D Brillouin zone of graphene. The parameters *t* and *s* are expressed in electron-volt units (eV), whereas *t* is given in nondimensional units. At the special points K and K of the graphene BZ the valence and conduction bands cross at the Fermi level (energy at 0 eV).

The traditional presentation of an electronic dispersion along the $K - \Gamma - M - K$ lines in Brillouin zone is given by selecting "usual" under "show Brillouin zone". Checking "show mesh" gives the distribution of

The hysteresis increases at larger ε for the graphene-coated aerogels. Insets: photographs of aerogels after graphene coating at $\varepsilon = 0\%$ (left) and 60% (right).

Optical properties

Graphene's ability to absorb a rather large 2.3% of white light is also a unique and interesting property, especially considering that it is only 1 atom thick. This is due to its aforementioned electronic properties; the electrons acting like massless charge carriers with very high mobility. A few years ago, it was proved that the amount of white light absorbed is based on the Fine Structure Constant, rather than being dictated by material specifics. Adding another layer of graphene increases the amount of white light absorbed by approximately the same value (2.3%). Graphene's opacity of $\pi \alpha \approx 2.3\%$ equates to a universal dynamic conductivity value of G=e2/4 \hbar (±2-3%) over the visible frequency range.

Due to these impressive characteristics, it has been observed that once optical intensity reaches a certain threshold (known as the saturation fluence) saturable absorption takes place (very high intensity light causes a reduction in absorption). This is an important characteristic with regards to the mode-locking of fibre lasers. Due to graphene's properties of wavelength-insensitive ultrafast saturable absorption, full-band mode locking has been achieved using an erbium-doped dissipative soliton fibre laser capable of obtaining wavelength tuning as large as 30 nm.

The optical properties of graphene are very unique. It shows Drude-like intraband conductivity followed at higher energies by a region of reduced conductivity before a sharp rise to a constant universal background value allowed states inside the bands representing the density of states function. Check "add

BZ and points" to see the location of high-symmetry points in BZ.

Setter bars under "show more detailed dispersion" let you compare the lattice electron behavior at the hyperbolic saddle M-point and quasi-linear (Dirac) dispersion curves at the K-points of BZ.

Snapshot 1: traditional representation of an electronic dispersion relation for the graphene along the $K - \Gamma - M - K$ lines of the first Brillouin zone.

Snapshot 2: pseudo-3D energy dispersion for the two π -bands in the first Brillouin zone of a 2D honeycomb graphene lattice.

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Snapshot 3: constant energy contours for the π -valence band and the first Brillouin zone of the grapheme.

Snapshot 4: same constant energy contours for the π^* -conduction band in an extended 3×3 Brillouin zone.

Snapshot 5: pseudo-3D energy dispersion for the π^* -conduction band at the saddle M-point (van Hove saddle point).



Snapshot 1

Equal to twice the value of the chemical potential. The linear bands near the Fermi level that result in an intraband Drude response and an interband plateau in the optical conductivity have been well described by optics experiments. However there are features that should be observable in optics. These features would originate from many-body effects and are believed to be dominated by electron-phonon interactions and electron-electron interactions. In *J. Phys.: Condens. Matter* **24**245601 we present proof-of-concept theoretical calculations in which we identify the impact of these many-body effects on optical conductivity and optical self-energies.

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Snapshot 2

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Snapshot 4

Figure 5 (a)Optical self-energy, and different calculations for the bosonic functions. EEI: electron–electron interaction; EPI electron–photon interaction.

The primary way in which this work differs from previous many-body calculations is our assumption of a boson-exchange model. Within this framework we can extract, using a maximum entropy inversion technique, a set of optically relevant spectra, including optical self-energies, scattering rates, and the underlying bosonic spectral density function, $\alpha^2 F(\omega)$

We find that electron–electron interactions produce chemical potential dependent features, which are rather flat and absent of structure. In contrast, the dominant optical phonon in graphene produces a clear peak which should be observable through the other background features. With these results in hand, a similar analysis of experimental data should provide clear indications of the relevant boson-exchange processes in graphene, their strength, as well as their chemical potential and substrate dependence.

Finally, our results in *J. Phys.: Condens. Matter* **24** 245601 also demonstrate the connection between the interband optical conductivity and the lower band of the quasiparticle spectral function, $A^{-}(k,\omega)$. Variations in the spectral function at energies just below the universal plateau onset can be used to isolate the interband conductivity from the intraband.

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Figure 5 (b) The carrier spectral density (solid green) for the lower Dirac cone at momentum $k = k_F$ as a function of normalized energy normalized by the chemical potential. The solid black curve gives the interband contribution to the graphene conductivity and its first derivative is given by the dashed blue curve.

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