



Structural Properties of Graphene

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Abstract

Graphene, a flat monolayer of carbon atoms tightly packed into a two-dimensional (2D) honeycomb lattice with six carbon atoms, are of two types due to their bonding. Due to its structural uniqueness, properties of the graphene is found to be very different and important in application point of view. Hence, the authors have studied the structural properties as co-ordination number, coordinates, distances of nearest atoms from 1st to 5th, analytically using two dimensional coordinate system taking one atom of a unit cell at the origin. Furthermore, packing fraction is also calculated, as the property is very important to study absorption/adsorption of different atoms into the sheet of it.

Key Words: *graphene, neighboring atoms, coordination number, packing fraction*

Introduction

Graphene is a flat layer of carbon atoms tightly packed in the form of a two-dimensional (2D) honeycomb lattice. It is a basic building block for graphitic. By peeling highly oriented pyrolytic graphite (HOPG), Novoselov and Geim presented an approach (Novoselov et al., 2004) for producing monolayer graphene in 2004. This experimental scotch tape method opened ability of formation of the 2D lattice and then for investigation of structure and various properties of graphene. Due to the exceptionally high crystal quality (Novoselov et al., 2005; Meyer et al., 2007) and massless Dirac fermions (Novoselov et al., 2005), graphene exhibits various unique properties such as anomalous half integer quantum Hall effect (Zhang et al., 2005), ultra-high intrinsic strength (Lee et al., 2008), remarkable optical properties (Blake et al., 2007; C. Casiraghi et al., 2007) superior thermal conductivity (Balandin et al., 2008) and extremely high charge carrier mobility (Novoselov et al., 2004; Morozov et al., 2008; Kim et al., 2009).

A single atomic layer of carbon i.e. graphene can be wrapped up into other graphitic materials with completely different structure and properties such as fullerene, carbon nanotubes, and thin graphene films (Geim et al., 2007). The 1st structure i.e. fullerene is the zero dimension (0D) structure. The 2nd structure i.e. nanotubes is the one dimension (1D) structure (Geim et al., 2007) and the 3rd structure, i.e. multilayer (only few layers) graphene is basically in the form of two dimensional (2D) structure. It can be monolayer, bilayer and few more layers too. It is the strongest material ever tested (Changgu et al., 2008; Cao et al., 2020).

A monolayer of graphene, has two carbon atoms in its unit cell are said to be A and B, as shown by solid blue and hollow magenta circles in the Figure 1. The bond angle between these atoms is 120° (Bena et al., 2009), i.e. angle made by ABA or BAB. For each triangle sublattice, vectors of the generating base can be written as $a_1 = \frac{3}{2}a \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix}$, $a_2 = \frac{3}{2}a \begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \end{pmatrix}$ where, $a \approx 1.42 \text{ \AA}$ (Menacho et al., 2018) However a single layer of it has atoms arranged in a hexagonal lattice (Geim et al., 2007; Peres et al., 2009) nanostructure (Poothanari et al., 2019). Due to its structural

uniqueness, properties of the graphene is found to be very different and important and has been studied for its wide range of applications, especially for carbon-based materials. Although graphene is a form of graphite i.e. integral part of 3D materials, does not exist in the free-state i.e. the self-standing state, hence, unstable with respect to that of, fullerenes and nanotubes. However, free-standing graphene was unexpectedly found as discussed above.

Hence, the authors have studied the structural properties of graphene analytically with simple geometry. In the work some important parameters such as coordination number and the distance between 1st to 5th neighbor are studies. In addition to that some fundamental parameters as packing density etc. are also calculated. The studies are considered to be important for further calculation of advance parameters, characterized the material and to study application of graphene in different area. As comparing the packing density with and without the adsorption/absorption of different atoms/molecules into the sheet of it, it can be used to make sensor of those atoms/molecules.

Theory

Graphene is a single layer of atoms of graphite. Atoms in it are bonded with sp² bond and are arranged in a regular hexagonal pattern called honeycomb lattice (Geim et al., 2007, Peres et al., 2009) as shown in Figure 1. The carbon-carbon bond length is nearly 0.142 nm, [16] is the distance between 1st neighbors. The distance between two nearest atoms are separated with a fixed distance is also called lattice constants. The constants are the pillar to form crystal structure and signature for unit cell. It is the smallest repeating unit in the space lattice which when repeated over and over produces the complete crystal lattice. Information of such crystal lattices and related parameters are very useful to study the physical properties as well as the physical phenomena of the materials for their application point of view. Hence, the coordination number and the distance between atoms ranging from 1st to 5th neighboring

atoms and with their coordinates are calculated at present, analytically.

Graphene, an allotrope of carbon with its 2D atomic crystal arranged in a hexagonal lattice has 6 carbon atoms (Geim et al., 2007, Peres et al., 2009). The carbon-atoms represented by sky solid blue sphere and magenta-hollow spheres in the Figure 1, are of two types due to their bonding. For convenience the atom at 'o' is taken at origin (0, 0). The d_1 , d_2 , and d_3 are the co-ordinates of first nearest neighboring atoms. Since 'a' is the carbon-carbon distance from the origin o (0, 0), the co-ordinates of d_1 ($\sqrt{3}a/2$, $a/2$), d_2 ($-\sqrt{3}a/2$, $a/2$) and d_3 (0, -a) are calculated with geometrically and using 2D coordinate system. Similarly, f_1 , f_2 , f_3 , f_4 , f_5 and f_6 are the co-ordinates of second nearest neighboring atoms with their co-ordinates f_1 ($\sqrt{3}a$, 0), f_2 ($\sqrt{3}a/2$, $3a/2$), f_3 ($-\sqrt{3}a/2$, $3a/2$), f_4 ($-\sqrt{3}a$, 0), f_5 ($-\sqrt{3}a/2$, $-3a/2$) and f_6 ($\sqrt{3}a/2$, $-3a/2$). The 3rd nearest neighboring atoms are at g_1 , g_2 and g_3 and their coordinates are g_1 (0, 2a), g_2 ($-\sqrt{3}a$, -a) and g_3 ($\sqrt{3}a$, -a). The 4th nearest neighbor atoms are at h_1 , h_2 , h_3 , h_4 , h_5 , h_6 , and the co-ordinates are h_1 ($3\sqrt{3}a/2$, $a/2$), h_2 ($\sqrt{3}a$, 2a), h_3 ($-\sqrt{3}a$, 2a), h_4 ($-3\sqrt{3}a/2$, $a/2$), h_5 ($-\sqrt{3}a$, -2a), h_6 ($\sqrt{3}a$, -2a) are respectively. The 5th neighboring atoms and their coordinates are p_1 ($\frac{3\sqrt{3}a}{2}$, $\frac{3a}{2}$), p_2 (0, 3a), p_3 ($\frac{-3\sqrt{3}a}{2}$, $\frac{3a}{2}$), p_4 ($\frac{-3\sqrt{3}a}{2}$, $\frac{-3a}{2}$), p_5 (0, -3a) and p_6 ($\frac{3\sqrt{3}a}{2}$, $\frac{-3a}{2}$). The detail calculation of which are given in the Appendix.

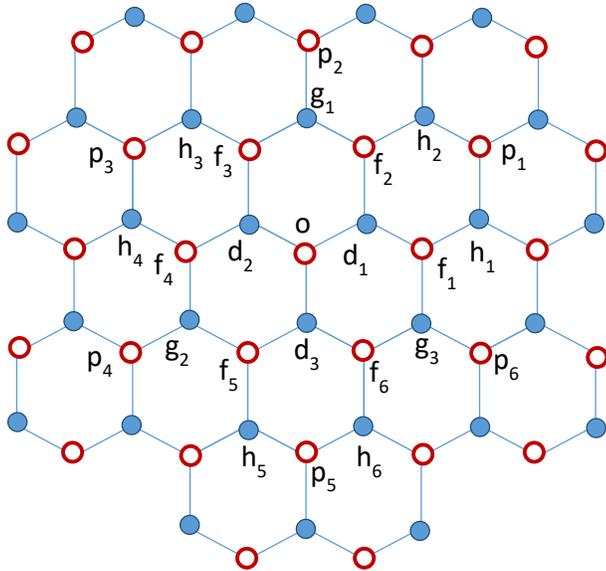


Figure. 1 A sheet of graphene, with the atom 'o' at the origin. d , f , g , h and p 's are the positions of 1st, 2nd, 3rd, 4th and 5th neighboring atoms. The distance of the 1st neighboring atoms are 'a=1.42 Å'.

Results and Discussion

Using geometry, some analytical structural properties of graphene is done such as finding of atomic co-ordinates,

coordinate numbers, distance of nearest atoms ranging from 1st to 5th and are given in the Table 1.

Figure 1 shows a sheet of graphene, in which an atom, 'o' is taken at the origin. d_1 , d_2 and d_3 are the positions of 1st neighboring atoms with the coordinates d_1 ($+\sqrt{3}a/2$, $a/2$), d_2 ($+\sqrt{3}a/2$, $-a/2$) and d_3 (0, -a). The distance of the 1st 3 neighboring atoms are calculated to be 1.42 Å.

Similarly, f_1 , f_2 , f_3 , f_4 , f_5 and f_6 are the positions of 2nd neighboring atoms; g_1 , g_2 and g_3 are the positions of 3rd neighboring atoms; h_1 , h_2 , h_3 , h_4 , h_5 and h_6 are the positions of 4th neighboring atoms and p_1 , p_2 , p_3 , p_4 , p_5 , and p_6 are the positions of the 5th neighboring atoms are at 2.45Å, 2.84 Å, 3.75Å and 4.26 Å respectively from the atom at 'o', the origin. The coordination numbers for 1st to 5th neighbor atoms are 3, 6, 3, 6 and 6 respectively, as given in the Table. 1. Gao Yang et al. have also calculated lattice constant and primitive lattice vectors as 1.42 Å, and 2:46 Å respectively (Yang et al., 2018).

Conclusions

The structural properties of graphene have been studied analytically. The number of neighboring atoms or coordination number of 1s to 5th are found to be, 3, 6, 3, 6, 6 respectively and are at distances 1.42Å, 2.45Å, 2.84Å, 3.75Å and 4.26 Å respectively. The coordinate of the neighboring atoms are also obtained. Packing fraction/density per unit hexagon is calculated to be 60%. The technique can be used to study the topological defect.

Table. 1: Table shows the co-ordinates and calculated distances for 1st, 2nd, 3rd, 4th and 5th nearest neighbors respectively, as shown in the Figure 1

neigh borin g atoms	Atoms from 'o'	Co-ordinates	Distance (Å)	Coordination No
1 st	d_1	$(\sqrt{3}a/2, a/2)$	a=1.42	3
	d_2	$(-\sqrt{3}a/2, a/2)$		
	d_3	$(0, -a)$		
2 nd	f_1	$(\sqrt{3}a, 0)$	$\sqrt{3}a = 2.45$	6
	f_2	$(\sqrt{3}a/2, 3a/2)$		
	f_3	$(-\sqrt{3}a/2, 3a/2)$		
	f_4	$(-\sqrt{3}a, 0)$		
	f_5	$(-\sqrt{3}a/2, -3a/2)$		
	f_6	$(\sqrt{3}a/2, -3a/2)$		
3 rd	g_1	$(0, 2a)$	2a=2.84	3
	g_2	$(-\sqrt{3}a, -a)$		
	g_3	$(\sqrt{3}a, -a)$		

4 th	h ₁	$(3\sqrt{3}a/2, a/2)$	$\sqrt{7}a=3.75$	6
	h ₂	$(\sqrt{3}a, 2a)$		
	h ₃	$(-\sqrt{3}a, 2a)$		
	h ₄	$(-3\sqrt{3}a/2, a/2)$		
	h ₅	$(-\sqrt{3}a, -2a)$		
	h ₆	$(\sqrt{3}a, -2a)$		
5 th	p ₁	$(\frac{3\sqrt{3}a}{2}, \frac{3a}{2})$	$3a=4.26$	6
	p ₂	$(0, 3a)$		
	p ₃	$(\frac{-3\sqrt{3}a}{2}, \frac{3a}{2})$		
	p ₄	$(\frac{-3\sqrt{3}a}{2}, \frac{-3a}{2})$		
	p ₅	$(0, -3a)$		
	p ₆	$(\frac{3\sqrt{3}a}{2}, \frac{-3a}{2})$		

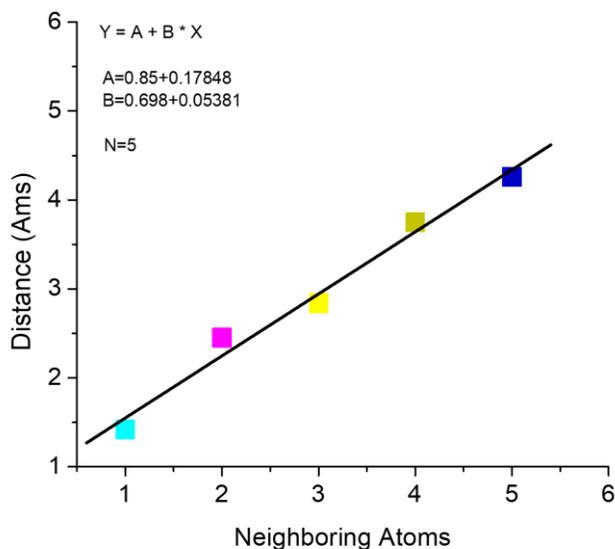


Figure 2: Variation of the atomic distances versus order of neighboring atoms from 1st to 5th of graphene. The fitted curve is a straight line with slope, $A=0.85$ and intercept on y axis $B=0.698$ with an error ± 0.17848 and ± 0.05381 respectively.

B. Conclusion and Future Work

The structural properties of graphene have been studied analytically. The number of neighboring atoms or coordination number of 1s to 5th are found to be, 3, 6, 3, 6, 6 respectively and are at distances 1.42Å, 2.45Å, 2.84Å, 3.75Å and 4.26 Å respectively. The coordinate of the neighboring atoms are also obtained. Packing fraction/density per unit hexagon is calculated to be 60%. The technique can be used to study the topological defect.

Future Work

The calculation can be extended for more order neighboring atoms. The calculated distances can be used to find the binding energy and nature of bonding etc. The obtained packing fraction value can be used to study absorption and adsorption of foreign atoms and molecules in it. The information can be used for making sensor of those atoms. Present and absence of displacement of lattices by such foreign atoms, can also be also be studied.

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Appendix

From the origin atom ‘o’,

1st 3 nearest neighboring atoms are at d₁, d₂, and d₃, at a distances ‘a’

2nd 6 nearest neighboring atoms are at f₁, f₂, f₃, f₄, f₅, and f₆ are at a distances ‘a√3’, is obtained as, $2\sin 60^\circ * a = \frac{\sqrt{3}a}{2}$

3rd 3 nearest neighboring atoms are at g₁, g₂, and g₃ are at a distances ‘2a’, is obtained as

$$= \sqrt{(\sqrt{3}a)^2 + a^2} = 2a$$

4th 6 nearest neighboring atoms are h₁, h₂, h₃, h₄, h₅, and h₆ are at a distances ‘3a’, is obtained as

5th 6 nearest neighboring 6 atoms are p₁, p₂, p₃, p₄, p₅, and p₆ are at a distances ‘√7a’, is obtained as

$$\sqrt{(\sqrt{3}a)^2 + (2a)^2} = \sqrt{7}a$$

Packing fraction = $2 * \frac{\pi^2}{4} * \frac{2}{3\sqrt{3}a^2} * 100\%$ (using a = 1.42Å)
 $= \frac{\pi}{3\sqrt{3}} * 100\% = 60\%$

$$PF = \frac{N_{particle} V_{particle}}{V_{unit\ cell}}$$