

LEARN MORE ABOUT BUCKY-BALL

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Carbon has been known as the king of elements because of its versatility and diversity in all areas. Currently, it has three allotropic forms viz., diamond, graphite and buckminsterfullerene (C_{60}) or bucky-ball, in short. Diamond has been prized for centuries as a gemstone of extraordinary beauty, brilliance and lustre. The word diamond derives its name from the alteration of the Latin word *adamas* meaning 'untamable' referring to its hardness. The name graphite comes from the greek verb *graphian* meaning 'to write'. It has been used in lubricants, seals, insulators, filters, refractors, electrodes and writing material. Bucky-ball, the third form of carbon, was synthesised in laboratory by Smalley and Kroto (1985). Scientists have been speculating that bucky-ball might be formed every time we light a candle. They have also suggested that it might be abundant in clouds of interstellar dust (Smalley, 1996). The properties associated with two allotropic forms (diamond and graphite) of carbon have already been investigated thoroughly and researchers are well aware of the properties of these two forms (Gopalkrishnan and Subramanyam, Dec. 2002) and (Ravichandran, Sept. 2001). However, regarding the third new form (bucky-ball) of carbon, there is very little

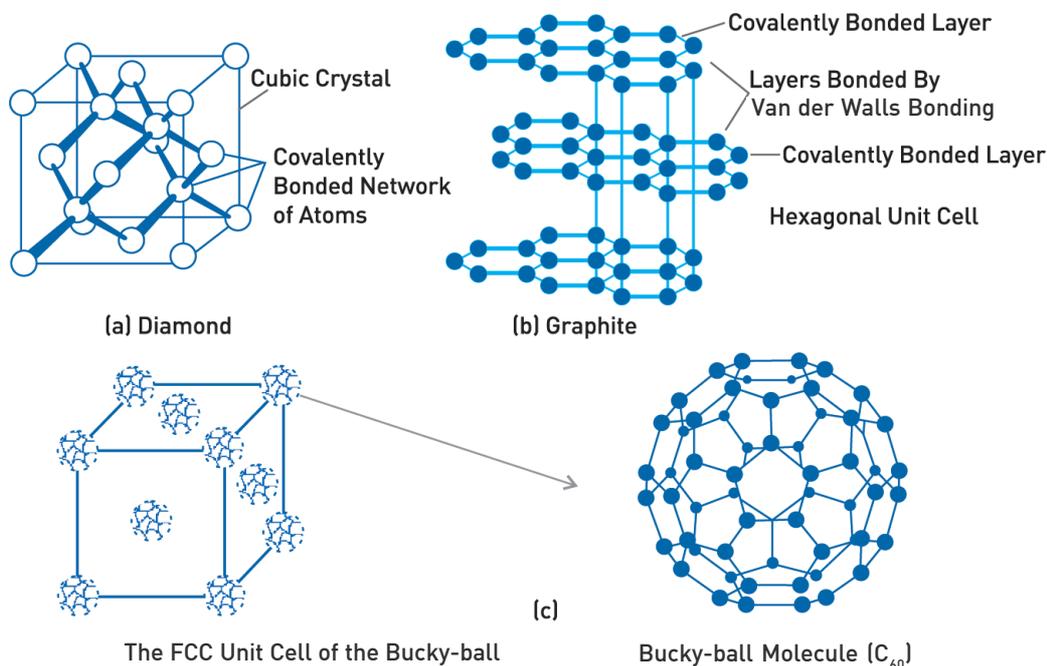
awareness among students till date. This has been realised during the supervision duty in internship programme of B.Sc. B.Ed. in different schools. Keeping the above in view, attempts have been made to highlight the properties and derivatives associated with the 'bucky-ball' and also to discuss its structural properties, synthesis methods and applications in this article.

Allotropic Forms of Carbon and their Structures

Carbon has three crystalline allotropic forms viz., diamond, graphite and bucky-ball. Their crystal structures are shown in Fig. 1(a), (b) and (c) respectively. Graphite is the carbon form that is stable at room temperature. Diamond is the stable form at very high pressures. Once formed, diamond continues to exist at atmospheric pressure and below about 900°C , because the transformation rate of diamond to graphite is virtually zero under these conditions. Graphite and diamond have widely differing properties, which lead to diverse applications (Table 1). For example, graphite is an electrical conductor whereas diamond is an insulator.

Table 1
Properties of three allotropic forms of Carbon

| Properties | Graphite | Diamond | Bucky-ball |
|------------|-------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------|
| Structure | Covalent bonding within layers, Van der Waals bonding between layers, Hexagonal crystal structure | Covalently bonded network. Cubic crystal structure | Covalently bonded C_{60} spheroidal molecules held in an face centred cubic crystal structure by Van der Waals bonding |
| Electrical | Good electrical conductor | Very good electrical insulator | Semiconductor compounds with alkali metal (e.g. K_3C_{60}) exhibit super-conductivity |
| Thermal | Thermal conductivity comparable to metals | Excellent thermal conductor, about five times more than Copper | |
| Mechanical | Lubricating agent, Mechanable. Bulk graphite $Y = 27 \text{ G Pa}$ $\bar{n} \sim 2.25 \text{ g cm}^{-3}$ | The hardest material $Y = 827 \text{ G Pa}$ $\bar{n} = 3.25 \text{ g cm}^{-3}$ except boron nitride | Mechanically soft. $Y = 18 \text{ G Pa}$ $\bar{n} = 1.65 \text{ g cm}^{-3}$ |



The bucky-ball (C_{60}) is the most symmetric molecule having icosahedral point group with 120 symmetry operations. It has a shape of a soccer ball in which 60 carbon atoms bond with each other to form a perfect soccer ball type molecule. This molecule has 12 pentagons and 20 hexagons, joined together to form a spherical molecule with each carbon atom at a corner as depicted in Figure 1 (c). It has been established that solid C_{60} forms a face centred cubic (F.C.C.) lattice with a lattice constant 14.17 \AA at room temperature. In this structure the distance between the nearest neighbour C_{60} cluster is 10 \AA and thus the intercluster separation is 2.9 \AA . Scanning tunneling microscope (Fig. 2 a and b) and scanning electron microscope (Fig.3) pictures clearly show the hexagonal arrays of closely packed spherical balls. (Grigoryan et. al. (1992), Sharma et. al. (1992), Kratschmer et. al. (1990) and Baggot (1991).) Table 2 provides x-ray diffraction parameters for a crystal of bucky-ball. The typical properties of bucky-ball are summarised in Table 3.

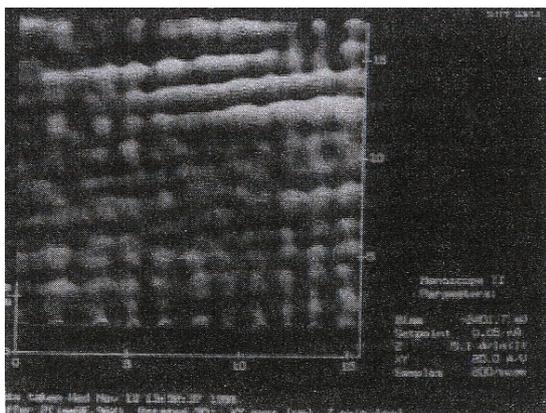


Fig. 2(a): Scanning tunneling micrograph of molecularly resolved buckyball image in 3D perspective. Bias voltage and current are shown in scanning tunneling micrograph.

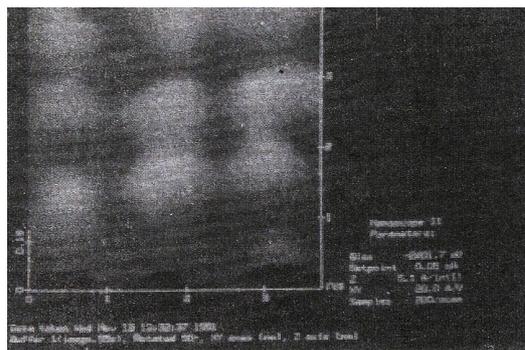


Fig. 2(b): Same micrograph at higher magnification

Table 2: X-ray diffraction parameters

| Measured 2θ (degree) | Measured d spacing (\AA) | Calculated d spacing (\AA) | Assignment miller indices (hkl) |
|-----------------------------|-------------------------------------|---------------------------------------|---------------------------------|
| 10.2 | 8.70 | 8.68 | (100) |
| 10.81 | 8.18 | 8.18 | (002) |
| 17.69 | 5.01 | 5.01 | (110) |
| 20.73 | 4.28 | 4.28 | (112) |
| 21.63 | 4.11 | 4.09 | (004) |
| 28.1 | 3.18 | 3.17 | (114) |
| 30.8 | 2.90 | 2.90 | (300) |
| 32.7 | 2.74 | 2.73 | (006) |

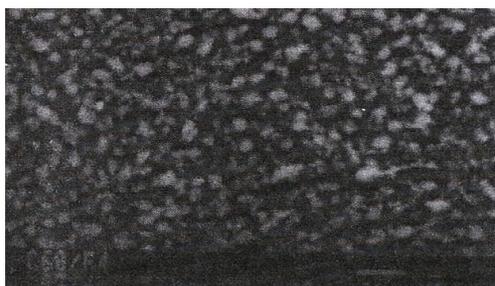


Fig. 3: Scanning electron micrograph of a film of bucky-ball. Magnification, scale and operating voltage are shown on the micrograph.

Table 3
Some properties of bucky-ball

| | |
|----------------------------------------------------------------------------|--------------------------------------------------------|
| Shape | Spherical (20 hexagons and 12 pentagons) |
| Dimensionality | 3D |
| Density | 1.7 g/cm ³ |
| Crystal structure | Face centered cubic |
| C - C bond length | 1.44 Å |
| State of Hybridisation | Intermediate between SP ² & SP ³ |
| Nearest neighbour distance | 10.04 Å |
| Diameter | 7.1 Å |
| Lattice parameter | 16.2 Å |
| Index of refraction | 2.2 |
| Infrared active modes | 1429, 1183, 577, 528 cm ⁻¹ |
| Bulk modulus | 18 giga Pascals |
| Ionisation potential | 7.6 eV |
| Cohesive energy for C ₆₀ molecule | 1.5 eV |
| Cohesive energy for atom | 7.4 eV |
| Electrical resistivity | 10 ¹¹ -10 ¹⁴ ohm |
| Magnetic susceptibility | 260 g ppm |
| Electron band gap | 1.5 eV |
| Effective mass of conduction band electron | 1.3 m _e |
| Superconducting transition temperatures for K ₃ C ₆₀ | 19K |
| Rb ₃ C ₆₀ | 29K |
| Cs ₂ Rb C ₆₀ | 33K |
| Rb _{2.7} Tl _{2.3} C ₆₀ | 42.5K |
| Colour | Black |
| Doping metal | Intercalation of alkali |

| | |
|-----------------------------------------------------------------------------------------------------------------------------|--------------------------|
| Coherence length | 100 Å |
| Penetration depth | 2000-4000 Å |
| Fermi energy (E _f) | 0.3 eV |
| V _f | ~ 2×10 ⁷ cm/s |
| Isotope effect | 0.3 – 1.2 |
| Critical magnetic field [H _{e2} (O)] | 50 tesla |
| Density of states [N (E _f) RB ₃ C ₆₀ /N(E _f) K ₃ C ₆₀] | 1.21 |
| 2Δ _B /K _B T _C | 5.3 |

Synthesis of Bucky-ball (C₆₀)

Synthesis of bucky-balls has been carried out by using mainly two techniques viz. (i) graphite arc welding, and (ii) laser ablation.

Graphite Arc Welding Technique

In this technique graphite rods of spectroscopic pure grade are butted together and a high current of the order of 100 amperes is passed through them in a controlled inert gas (He/Ar) atmosphere. The apparatus consists of a vacuum chamber, which is evacuated and then filled with inert gas (He). To the evaporated graphite condenses on the inner surface of a glass cylinder surrounding the graphite electrodes from which it is scrapped off. It has been noticed that the He pressure is very crucial for optimising the yield of bucky-ball (C₆₀). By this method solid C₆₀ is prepared in the form of graphite soot. The C₆₀ has been separated from the soot using liquid chromatography.

Laser Ablation

Laser ablation deposition technique has also been used to prepare the C_{60} films. In this technique, the laser beam enters the vacuum chamber through a window and is focused on a target of graphite of spectroscopic pure grade. During evaporation under the energy of the laser beam, the emitted matter forms a plume that carries the vaporised graphite to the substrate. The process works in very high vacuum as well as in inert atmosphere. By this technique very good quality homogeneous films of bucky-balls have been prepared.

Properties of Bucky-ball

Chemical properties of bucky-ball have depicted that it is a highly stable molecule. Ion beam experiments with 250 eV impact energy have shown high inelasticity of the ions but gave no evidence of impact induced fragmentation. Bucky-ball possesses a vanishingly small δ -electron ring current and hence has magnetic susceptibility far below that of graphite or benzene.

Electrochemical studies have proved that bucky-ball is very strong oxidising agent and does not react with electrophiles. Rather it is easily reduced and reacts readily with nucleophilic agents like alkali metals.

Superconductivity in Bucky-ball

Bucky-ball (C_{60}) doped with potassium formed a new metallic phase known as 'buckide' and

resulted in its maximum electrical conductivity when there were three potassium atoms intercalated to each bucky-ball. If too much potassium is added, however, the material becomes insulating. K_3C_{60} , a metal, becomes a superconductor when cooled below 18K. When rubidium was substituted for potassium, the critical temperature (T_c) was found to be 30K. Recently, superconductivity at 42.5K for rubidium-thallium doped material has been reported.

Derivatives of Bucky-ball

The synthesis of bucky-balls C_{60} to C_{266} in very high yield (upto 44% extractable) by plasma discharge technique has been reported by Parker *et. al.* (1991). They have characterised the extracted samples by time of flight mass spectrometry and Fourier transform mass spectrometry and concluded that almost one-third of the extractable material is composed of bucky-balls C_{84} to C_{200} (Parker *et. al.* 1991). Similar to discovery of bucky-ball, a major breakthrough came in 1991 when the synthesis of carbon nano tubes (CNTs) was announced by Iijiyama. Careful analysis revealed that these carbon nano tubes are long tubes made from a planar sheet of graphite that is wrapped into a seamless tube, nanometer in diameter and few microns in length. They are very stable and found to be good yield emitters and can be operated at lower electric field giving larger currents (Purandare and Patil, 2002).

Future Projection and Application of Bucky-ball

Bucky-ball research has immense scope in nanoscience and technology. The most technologically interesting property of bulk bucky-ball is electronic in various forms of the compound. Since, By playing with the doping concentration of alkali-metal, it functions as an insulator, conductor, semi-conductor and super-conductor. Bucky-ball and its derivatives and CNTs can be the potential source of use in catalytic chemistry, bimolecular recognition, nanoreactors, flat panel display technology, electron microscope and atom force microscopy. Also it can be used as molecular sieves and also as inhibitions to the activity of HIV virus. Some scientists even believe that the silicon technology may be replaced in future by bucky-balls cluster based devices.

Conclusion

The bucky-ball, hollow cage-shaped huge molecule composed of 60 carbon atoms (the third crystalline allotropic form of carbon after well known diamond and graphite), started to attract an increasing attention of scientific community. The existence of higher derivatives (C_{60} to C_{266}), synthesised by the time-of-flight mass spectroscopy and Fourier transform mass and spectrometry. In future, the bucky-ball and its higher derivatives including carbon nano tubes can be considered as potential candidates for applications in electronics, nanoscience, atom force microscopy, catalytic chemistry, etc. In particular, the occurrence of superconductivity in alkali metal doped bucky-ball continues to be a fascinating aspect of bucky-ball.

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