CARBON NANOTUBES

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1. Introduction

We've heard a lot about graphene this semester, but let's now consider carbon nanotubes (CNTs). Just like diamond and graphene, CNTs are an allotrope of carbon. CNTs can be regarded as rolled up graphene, as can be seen on the slide. They exist in single-walled (SWCNT) and multi-walled (MWCNT) variants. But among these types, multiple configurations are also possible by "rolling" the graphene differently. This presentation will be a brief description of what CNTs is, what kinds there are, what the electronic structure is, how it's produced, and what we can do with it.

2. Configurations

Besides the single-walled and multi-walled variants, CNTs exist in multiple configurations depending on how the graphene is stitched to itself. To see this, imagine an unrolled CNT, i.e. a sheet of graphene with finite width (with some limitations). The sheet consists of two triangular sublattices A and B of which B is rotated 60 degrees with respect to A. The carbon atoms in graphene have each three bonds with directions depending on their sublattice. To construct a CNT, take a lattice point to start with, call it a. To be able to roll the CNT, we have to find a lattice point b in the same sublattice as a, and roll the sheet so that a and b match. The vector connecting a and b we call $\vec{w}$. The original lattice has to be cut along lines perpendicular to $\vec{w}$ and intersecting with a and b respectively. This vector $\vec{w}$ can be written as linear combination of basis vectors $\vec{u}$ and $\vec{v}$ for the graphene sublattice as $\vec{w} = n \cdot \vec{u} + m \cdot \vec{v}$. In this way, one configuration of CNT is determined by a pair (n, m). Note that (n, m) is the same as $(-2m, n + m)$, which is rotation by 60 degrees. Also not all pairs are possible, as there need to be enough atoms to create a tube. The circumference of a CNT of type (n, m) is given by the length of $\vec{w}$, i.e. $|\vec{w}| = |\vec{u}|\sqrt{n^2 + nm + m^2}$ with $|u| \approx 246\,\text{pm}$.

2.1. Common classifications.

Common classifications are (for $k \neq 0$):

- **Zigzag** $(k, 0)$ or $(0, k)$
- **Armchair** (k, k)
- **Chiral** (n, m) with $m > 0, n \neq m$

2.2. Chiral nanotubes.

Like stereoisomers, all nanotubes exist in two different chiralities, except for the zigzag and armchair CNTs. For types (n, m) with $m > 0, n \neq m$, we call its mirror image its enantiomer: a nanotube of type (m, n).

3. Properties

Most of the electronic structure is inherited from graphene, such that CNTs are expected to have impressive electronic, thermal, and mechanical properties. A good, thorough read with lots of examples can be found in [4]. $(2, 2)$ is the thinnest type of CNT with a diameter of 0.3 nm. Due to sp^2 hybridized bonds, the single-walled tubes are very strong, while remaining thin. In comparison, SWCNTs are at least 23 times stronger (tensile) than steel[1]. As CNTs are very thin, CNT materials are light.

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What is most interesting for the theoreticians, is the electronic structure.[1] The classification as proposed in the former section, yields some distinction in the electronic behaviour of these types. Unlike graphene, CNTs aren't semimetallic. Zigzag and armchair CNTs are achiral and those are mostly metallic, and chiral CNTs are mostly semiconductor. One example of a deviation from this, is $(8, 2)$.[4] Although the material is achiral, there is no band gap. There is a rule that a CNT is metallic if $3|(n - m)$.

4. Applications

A lot of research into CNTs is going on. There are many promising ideas. The past decades, CNTs were extensively analysed by theoreticians, such as our own Misha Katsnelson. But the properties have also been put into practice.[3] In materials, CNTs are used as an additive to add properties, such as electrical conductivity, tensile strength, better thermal conductivity. They are also used on their own, for example to create long fibres for fabric.

In chemistry, CNTs can be used as catalysts. Reactants bond to a CNT loosely, but the electronic structure can change such that reactions are easier. One caveat, however, is that different types of CNT behave differently, and type pure CNT batches are not easy to produce.

As many CNTs are semiconducting, one obvious candidate for application is in transistors.[2] Even at sub-10 nm scale, transistors are possible, thus offering a good alternative to silicon, as the struggle to decrease chip size continues.

5. Conclusion

Carbon nanotubes are a very versatile class of molecules. A lot has been researched, but a lot is yet to uncover. On the application side, there is are lot of ideas.

For SWCNTs, most properties can be found in the class of CNT by distinguishing zigzag, armchair, and chiral types. Recognizing their differences - along with the $3|(n - m)$ rule - enables one to do a good guess about its properties. Combining CNTs into MWCNTs creates metallic structures, although they are mostly only Van der Waals bound.

The future brings a lot of opportunities. Questions like whether CNTs are superconductors or whether they will revolutionize computing are still unanswered.

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For more theoretic information, see [5] for a good overview of the development of graphene and CNTs, or [4] for some more examples. I can also recommend reading [3] for more about applications.

References

[1] Nanotubes for Electronics. *Scientific American*, 12 2000.
[2] 20 years of nanotube transistors. *Nature Electronics*, 1(3):149–149, Mar. 2018.
[3] M. Berger. Carbon nanotubes – what they are, how they are made, what they are used for, 2021.
[4] S. M.-M. Dubois, Z. Zanolli, X. Declerck, and J.-C. Charlier. Electronic properties and quantum transport in Graphene-based nanostructures. *The European Physical Journal B*, 72(1):1–24, Nov. 2009.
[5] A. K. Geim and K. S. Novoselov. The rise of graphene. *Nature Materials*, 6(3):183–191, Mar. 2007.

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[1] Andre Geim, one of the pioneers of graphene extraction (from graphite), tends to defend graphene as not being "only an academic material".