BS PAS 134 (2012) (English): Terminology for carbon nanostructures

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PAS 134:2012

BSI Standards Publication

Terminology for carbon nanostructures

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ISBN 978 0 580 75665 8

ICS 01.040.71; 71.100.99

The following BSI references relate to the work on this standard:

Publication history

First edition published 2007
Second (present) edition, March 2012

Amendments issued since publication

Date	Text affected

Contents

Annexes

Summary of pages

This document comprises a front cover, an inside front cover, pages i to ii, pages 1 to 16, an inside back cover and a back cover.

Foreword

Publishing information

This Publicly Available Specification (PAS) was commissioned by the Departement for Business, Innovation and Skills (BIS) and its development was facilitated by the British Standards Institution (BSI). It came into effect on 23 March 2012.

Acknowledgement is given to the following organizations that were involved in the revision of this terminology as members of the Steering Group:

Cranfield University;

Ionbond UK Ltd;

National Physical Laboratory;

University of Cambridge.

In addition, acknowledgement is given to the contributions of those that commented, including BSI Technical Committee NTI/1, *Nanotechnologies*, the working groups of ISO Technical Committee ISO/TC 229, *Nanotechnologies*, and other organizations and experts.

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The PAS process enables a specification to be rapidly developed in order to fulfil an immediate need in industry. A PAS may be considered for further development as a British Standard, or constitute part of the UK input into the development of a European or International Standard.

Relationship with other publications

This PAS is issued as part of a suite of nanotechnology terminology PASs:

- PAS 71, *Vocabulary – Nanoparticles;*
- PAS 131, *Terminology for medical, health and personal care applications of nanotechnologies*;
- PAS 132, *Terminology for the bio-nano interface*;
- PAS 133, *Terminology for nanoscale measurement and instrumentation*;
- PAS 134, *Terminology for carbon nanostructures*;
- PAS 135, *Terminology for nanofabrication*;
- PAS 136, *Terminology for nanomaterials*.

Contractual and legal considerations

This publication does not purport to include all the necessary provisions of a contract. Users are responsible for its correct application.

Compliance with a Publicly Available Specification cannot confer immunity from legal obligations.

Introduction

The first edition of this Publicly Available Specification (PAS) was, along with five other vocabulary documents, commissioned by the UK Department of Trade and Industry (DTI) in 2006 for the purposes of developing and encouraging the use of a common language relevant to nanotechnologies and nanomaterials. These PASs were intended to seed, and have seeded, further developments and discussions in formal standards-making. They have informed the preparation of other standards in this area.

Nanotechnologies are a group of emerging technologies, characterized by the "application of scientific knowledge to manipulate and control matter in the nanoscale in order to make use of size- and structure-dependent properties and phenomena, as distinct from those associated with individual atoms or molecules or with bulk materials" (see DD ISO TS 80004-1:2012, definition **2.3)**. These technologies are evolving quickly and will gain increasing importance over the next few years. Their application is expected to impact virtually all areas of human endeavour, in particular agriculture, construction, energy generation and storage, engineering, environmental remediation, healthcare, ICT, medicine and medical devices, pharmaceuticals, sustainability and transport.

This PAS was commissioned in response to demands by UK industry to provide standards to support future applications. The intention was to bring together the disparate terms and definitions relevant to carbon nanostructures and their production, measurement and characterization.

The principal difference between a PAS and a full British, European or international standard, is that a PAS is created in a consultative process across industry rather than gaining the full consensus of a specific technical committee.

The remit of this PAS is to document and, to a lesser degree, comment on the current use of basic carbon nanostructure terms and definitions in use by manufacturers, suppliers, academia, regulators and governments, and to make recommendations for usage as required. It also includes terms defining production methods and analytical techniques employed by those working with carbon nanomaterials.

Together with six related PAS vocabularies,¹⁾ PAS 134 has helped to stimulate international activity in the area being undertaken by a joint working group between ISO/TC 229, *Nanotechnologies*, and IEC/TC 113, *Nanotechnology standardization for electrical and electronic products and systems*. This activity has so far contributed to the publication of five internationally accepted vocabularies, the relevant output of which is reflected in this revision of PAS 134, in particular that contained in DD ISO TS 80004-3:2010, *Nanotechnologies – Vocabulary – Part 3: Carbon nano-objects*. While it was the intention to withdraw this PAS once equivalent full consensus international standards on the subject have been published, the scope of DD ISO TS 80004-3 is limited to terms specific to carbon nano-objects and does not include the wider remit of terms covered in the present document. Hence it was decided that PAS 134 should be revised to align relevant terms with the ISO documents but that it should be maintained until such time as its scope is completely addressed by other publications.

This PAS does not provide a nomenclature system for carbon nanostructures, as this is a specialized subject and there is no current consensus in the nanotechnologies or nanosciences communities on how to approach such a system for the collection of carbon nanostructures, although work has commenced in ISO/TC 229 on developing a framework for nomenclature models for nano-objects.

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1) See www.bsigroup.com/nano

However, IUPAC[2] has developed a numbering system for one group of carbon nanostructures, the fullerenes [1], together with a nomenclature for a subset of these [2].

This vocabulary attempts not to include terms that are used in a manner consistent with a definition given in the *Oxford English Dictionary* [3], and terms that already have well established meanings to which the addition of the prefix "nano" changes only the scale to which they apply but does not otherwise change their meaning.

The multidisciplinary nature of nanotechnologies can lead to confusion as to the precise meaning of some terms because of differences in usage between disciplines. Users are advised that, in order to support the standardization of terminology, this PAS provides single definitions wherever possible.

1 Scope

This Publicly Available Specification (PAS) lists terms and definitions used in or associated with the chemical and physical structure, characterization, functionalization, manufacture and synthesis of carbon nanostructures.

It is applicable to, but not limited to, diamond, graphite, fullerene, nanofibre, nanohorn, nanorod, nanotube and graphene structures.

This PAS is intended for use by technologists, regulators, non-government organizations (NGOs), consumer organizations, members of the public and others with an interest in the application or use of nanotechnologies in the subject area.

2 General terms referring to nano-objects

2.1 nanocone

cone-shaped **nanofibre** or **nanoparticle**

[DD ISO/TS 80004-3:2010, definition **2.9**]

2.2 nanofibre

nano-object with two similar external dimensions in the **nanoscale** and the third dimension significantly larger

*NOTE 1 A **nanofibre** can be flexible or rigid.*

NOTE 2 The two similar external dimensions are considered to differ in size by less than three times and the significantly larger external dimension is considered to differ from the other two by more than three times.

*NOTE 3 The largest external dimension is not necessarily in the **nanoscale**.*

[DD CEN ISO/TS 27687:2009, definition **4.3**]

2.3 nano-object

material with one, two or three external dimensions in the **nanoscale**

*NOTE Generic term for all discrete **nanoscale** objects.*

[DD CEN ISO/TS 27687:2009, definition **2.2**]

2.4 nano-onion

spherical **nanoparticle** with concentric multiple shell structure

[DD ISO/TS 80004-3:2010, definition **2.8**]

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[2] International Union of Pure and Applied Chemistry.

2.5 nanoparticle

nano-object with all three external dimensions in the **nanoscale**

*NOTE If the lengths of the longest to the shortest axes of the **nano-object** differ significantly (typically by more than three times), the terms **nanofibre** or **nanoplate** are intended to be used instead of the term nanoparticle.*

[DD CEN ISO/TS 27687:2009, definition **4.1**

2.6 nanoplate

nano-object with one external dimension in the **nanoscale** and the two other external dimensions significantly larger

NOTE 1 The smallest external dimension is the thickness of the nanoplate.

*NOTE 2 The two significantly larger dimensions are considered to differ from the **nanoscale** dimension by more than three times.*

*NOTE 3 The larger external dimensions are not necessarily in the **nanoscale**.*

[DD CEN ISO/TS 27687:2009, definition **4.2**]

2.7 nanoribbon

nanoplate with one of its two larger dimensions in the **nanoscale** and the other significantly larger

[DD ISO/TS 80004-3:2010, definition **2.10**]

2.8 nanorod

solid **nanofibre**

[DD CEN ISO/TS 27687:2009, definition **4.5**]

2.9 nanoscale

size range from approximately 1 nm to 100 nm

NOTE 1 Properties that are not extrapolations from larger size will typically, but not exclusively, be exhibited in this size range.

*NOTE 2 The lower limit in this definition (approximately 1 nm) has no physical significance but is introduced to avoid single and small groups of atoms from being designated as **nano-objects** or elements of nanostructures, which might be implied by the absence of a lower limit.*

[DD CEN ISO/TS 27687:2009, definition **2.1**]

2.10 nanotube

hollow **nanofibre**

[DD CEN ISO/TS 27687:2009, definition **4.4**]

3 General terms relevant to carbon chemistry and carbon nanostructures

3.1 carbon hybridization

merging of the outer *s* and *p* orbitals in carbon atoms

NOTE Carbon has four valence electrons. In an isolated carbon atom, two of the valence electrons are expected to be in the 2s orbital and the other two to be in two of the three 2p orbitals. However, depending on the local conditions, one of the 2s electrons may move to the third 2p orbital allowing the 2s to merge with the 2p and form new kinds of orbital called sp. Even though the s and p orbitals are symmetric with respect to the nucleus of the carbon atom, the sp orbitals are highly directional and most of the electron cloud exists on one side of the carbon nucleus. sp^1, sp^2 *and* sp^3 *below are used to denote the different possible hybridizations in carbon.*

3.2 carbon nanotube (CNT)

nanotube composed of carbon

NOTE *Carbon nanotubes* *usually consist of curved* ***graphene*** *layers, including* ***single-wall carbon nanotubes*** *and* ***multiwall carbon nanotubes****.*

[DD ISO/TS 80004-3:2010, definition **4.3**]

3.3 fullerene

molecule composed solely of an even number of carbon atoms, which form a closed cage-like fused-ring polycyclic system with 12 five-membered rings and the rest six-membered rings

NOTE 1 Adapted from the definition in the IUPAC Compendium of Chemical Terminology [4].

NOTE 2 A well-known example is C_{60}*, which has a spherical shape with an external dimension of about 1 nm.*

[DD ISO/TS 80004-3:2010, definition **3.1**]

3.4 graphene

single layer of carbon atoms with each atom bound to three neighbours in a honeycomb structure

NOTE It is an important building block of many carbon ***nano-objects****.*

[DD ISO/TS 80004-3:2010, definition **2.11**]

3.5 heptagonal and pentagonal defects

interruption of the structure of graphitic layers with either heptagonal or pentagonal rings of carbon respectively

NOTE Carbon atoms in graphite are organized in hexagons; when one carbon atom is added or removed heptagonal or pentagonal defects are formed, respectively.

3.6 sp^1 carbon hybridization

merging between the 2*s* and one 2*p* orbitals

NOTE The two sp orbitals lie opposite to each other and on a straight line. Hybridization in linear chains of carbon atoms.

3.7 sp^2 carbon hybridization

merging between the 2*s* and two 2*p* orbitals

NOTE The three sp orbitals lie on the same plane at 120° from each other. Carbon atoms in ***graphene*** *are* sp^2 *hybridized.*

3.8 sp^3 carbon hybridization

merging between the 2*s* and all three 2*p* orbitals

NOTE The four sp orbitals point to the apexes of a tetrahedron. Diamond is made of sp^3 *hybridized carbon.*

3.9 turbostratic carbon

disordered graphitic structure where the graphitic planes may be distorted

4 Diamond nanostructures

4.1 Synthesis

4.1.1 detonation

method of producing nanoscale diamond material by use of a high pressure shock wave

NOTE Detonation initiates the shock wave.

4.1.2 high pressure high temperature (HPHT)
synthesis method using high temperature and pressure applied to a material held between two anvils to modify the material structure

NOTE This method is currently used to convert sp^2 bonded carbon into diamond.

4.1.3 hot filament chemical vapour deposition (HFCVD)
industrial synthesis method in which reactant gases are passed over a hot filament and deposit to form large area growth of, especially, polycrystalline and nanocrystalline diamond

4.2 Materials

4.2.1 adamantane
$C_{10}H_{16}$ closed structure comprising four benzene rings with hydrogen termination

NOTE The smallest member of the H-terminated, cubic diamond molecular series.

4.2.2 diamondoid
linked cages of **adamantane**

4.2.3 hydrogenated nanodiamond
H-terminated nanoscale diamond

4.2.4 ultradispersed diamond (UDD)
isolated diamond nanoparticles

*NOTE Typically produced by **detonation** synthesis.*

5 Carbon nanofibres – nanorods and nanotubes

5.1 Synthesis

5.1.1 arc discharge
use of an electric arc, formed by passing a high current between electrodes (in this case, usually graphite/carbon), to vaporize the electrode material and create a plasma

*NOTE This is a technique for producing **carbon nanotubes** and **nano-onions, amorphous carbon** and **diamond-like carbon** film deposition.*

5.1.2 base-growth mode
growth mode of carbon nanorod catalysed by a particle anchored on a support surface

NOTE Carbon feedstock is supplied from the base where the growing nanorod interfaces with the anchored catalyst.

5.1.3 chemical vapour synthesis (CVS)
gas phase synthesis where vapour is formed in a reaction chamber and condenses to form particles

NOTE 1 Also referred to as chemical vapour growth.

NOTE 2 The vapour can be formed by, for example, pyrolysis, reduction, oxidation or nitridation.

NOTE 3 One application is the synthesis of carbon nanotubes.

[PAS 71:2011 definition **6.5**]

5.1.4 gas phase synthesis

production method based on nucleation of a supersaturated vapour and subsequent particle growth by condensation, coagulation and coalescence

NOTE Examples include ***chemical vapour synthesis (CVS)****, furnace flow processing, laser pyrolysis,* ***physical vapour synthesis (PVS)*** *and plasma processing.*

[PAS 71:2011 definition **6.14**]

5.1.5 laser ablation processing

physical vapour synthesis using the energy from a (typically pulsed) laser beam to evaporate material from the surface of a target

NOTE 1 Also called laser assisted ablation.

[PAS 71:2011 definition **6.16**]

NOTE 2 Used with a graphite target to create a carbon plume, this is a precursor for growth of ***amorphous carbon*****,** ***diamond-like carbon*****,** ***carbon nanotubes****, or* ***fullerenes****.*

5.1.6 liquid arc synthesis

arc discharge carried out in a liquid environment

NOTE 1 For example, in water or liquid nitrogen.

NOTE 2 When operated with carbon electrodes this technique provides a rich source of high quality ***carbon nanotubes****.*

5.1.7 physical vapour synthesis (PVS)

gas phase synthesis where the vapour is formed by either heating a source material or bombarding it with energetic atoms, ions or molecules

NOTE 1 Heating may occur by indirect heating through contact with a hot surface, or direct heating using an electric arc, a beam of enegetic electrons, a laser beam, etc.

NOTE 2 The generation of vapour by bombardment with energetic atoms, ions or molecules is called sputtering.

5.1.8 template growth

growth of nanofibres/nanotubes where their direction is guided by some physical template

5.1.9 tip-growth mode

nanotube lengthening involving the removal of the catalyst particle from the support and its transportation to the open end of the tube where it continues to catalyse tube growth

NOTE Operates when the catalyst-support interaction is weak.

5.2 Materials

5.2.1 armchair carbon nanotube

nanotubes with chiral vector n = m

NOTE See ***chiral vector of single-wall carbon nanotube****.*

5.2.2 carbon nanohorn

short and irregular shaped **carbon nanotube** with a **nanocone** apex

NOTE Usually hundreds of carbon nanohorns constitute an aggregate nanoparticle.

[DD ISO/TS 80004-3:2010, definition **4.10**]

5.2.3 carbon nanopeapod

linear array of **fullerenes** enclosed in a **carbon nanotube**

NOTE This is an example of a composite ***nanofibre****.*

[DD ISO/TS 80004-3:2010, definition **4.9**]

5.2.4 chiral vector of single-wall carbon nanotube

vector notation used to describe the helical structure of a **single-wall carbon nanotube**

[DD ISO TS 80004-3:2010, definition **4.5**]

*NOTE 1 Described using the chiral vector, Ch = n x a1 + m x a2, which connects two crystallographically equivalent sites on the **graphene** sheet (where a1 and a2 are unit vectors from an atom to the next nearest neighbouring atoms in the regular hexagonal honeycomb lattice, and n and m are integers). Each **nanotube** topology is usually characterized by these two integer numbers (n, m), thus defining some peculiar symmetries such as **armchair** (n, n) and **zigzag** (n,0) classes.*

NOTE 2 The chirality of a nanotube determines its electronic properties, i.e. metallic or semiconducting.

5.2.5 cup-stacked carbon nanotube

carbon nanotube composed of stacked truncated **graphene nanocones**

*NOTE This is completely different from **single-wall** or **multiwall carbon nanotubes** in structure. The open top and bottom edges of truncated **graphene nanocones** appear on the inner and outer surfaces of the **nanotube**, respectively.*

[DD ISO/TS 80004-3:2010, definition **4.8**]

5.2.6 double-wall carbon nanotube (DWCNT)

multiwall carbon nanotube composed of only two nested, concentric **single-wall carbon nanotubes**

*NOTE Although this is a type of **multiwall carbon nanotube**, its properties are rather closer to **single-wall carbon nanotubes**.*

[DD ISO/TS 80004-3:2010, definition **4.7**]

5.2.7 graphitic nanofibre

carbon nanofibre composed of **graphene** multilayer structures

***NOTE** **Graphene** layers can have orientation with respect to the fibre axis without long-range order.*

[DD ISO/TS 80004-3:2010, definition **4.2**]

5.2.8 multiwall carbon nanotube (MWCNT)

carbon nanotube composed of nested, concentric or near-concentric **graphene** sheets with interlayer distances similar to those of graphite

*NOTE The structure is normally considered to be many **single-wall carbon nanotubes** nesting each other, and would be cylindrical for small diameters but tends to have a polygonal cross-section as the diameter increases.*

[DD ISO/TS 80004-3:2010, definition **4.6**]

5.2.9 single-wall carbon nanotube (SWCNT)

carbon nanotube consisting of a single cylindrical **graphene** layer

NOTE The structure can be visualized as a graphene sheet rolled into a cylindrical honeycomb structure.

[DD ISO/TS 80004-3:2010, definition **4.4**]

5.2.10 zigzag carbon nanotube

nanotube with chiral vector (n, 0).

NOTE Such a tube has mirror symmetry with respect to a plane that includes its axis.

6 Carbon films

6.1 Synthesis

6.1.1 cathodic vacuum arc deposition

physical vapour deposition technique using a **vacuum arc** on a carbon cathode to produce a high temperature carbon plasma which condenses on a substrate to produce a film

NOTE This is a type of ***arc discharge****.*

6.1.2 chemical vapour deposition (CVD)

chemical vapour synthesis in the presence of a substrate to produce a film

6.1.3 electron cyclotron resonance (ECR) CVD

technique using a low pressure, high density plasma generated by a microwave coupled with a magnetic field to promote chemical dissociation of carbon-containing gases to provide a source of excited carbon atoms for film formation on a substrate

NOTE This is a type of ***plasma-enhanced chemical vapour deposition****.*

6.1.4 electron cyclotron wave resonance (ECWR) source

high density plasma source for **plasma-enhanced chemical vapour deposition** comprising a single-turn inductively-coupled radio frequency discharge with static transverse magnetic field

NOTE This is typically used in the preparation of ***amorphous carbon*** *and* ***diamond-like carbon*** *thin films.*

6.1.5 filtered cathodic vacuum arc (FCVA)

vacuum arc source incorporating a magnetic and/or mechanical filter to provide a coating flux that is essentially free of macroparticles

NOTE One possible realization is the ***s-bend filter*** *using two curved toroidal filters, widely used for the deposition of* ***tetrahedral amorphous carbon*** *films.*

6.1.6 physical vapour deposition (PVD)

physical vapour synthesis in the presence of a substrate to produce a coating

6.1.7 plasma-enhanced chemical vapour deposition (PECVD)

chemical vapour deposition where the gas is decomposed using a plasma

*NOTE The plasma can be generated using direct current (DC-****PECVD****), radio frequency (RF-****PECVD****) or microwave (MW-****PECVD****) energy. This is a common technique for synthesizing* ***amorphous carbon, diamond-like carbon, carbon nanotubes*** *and diamond.*

6.1.8 s-bend filter

high efficiency filter for **vacuum arc** deposition using two curved toroidal filters

NOTE The filtering can be improved by a factor of 100 by adding baffles along the filter section.

6.1.9 sputter deposition

physical vapour deposition technique in which energetic particles, typically gas ions formed in a plasma, bombard a target material which is eroded and transferred (sputtered) onto another surface

NOTE This is a common industrial process for the deposition of ***amorphous carbon*** *and* ***DLC****. Amorphous hydrogenated carbon (a-C:H) can be produced by reactive sputtering of a carbon target using a plasma of argon together with hydrogen or methane.*

6.1.10 subplantation

process in which atoms are implanted into a material to produce densification

NOTE This term is typically used to describe the growth mechanism of ***DLC****.*

6.1.11 **vacuum arc**
arc discharge sustained in a vacuum

6.2 Materials

6.2.1 **amorphous carbon**
carbon material without long-range crystalline order

NOTE Short-range order exists, but with deviations of the interatomic distances and/or interbonding angles with respect to the graphite lattice as well as to the diamond lattice.

[Adapted from IUPAC Compendium of Chemical Terminology [4]]

6.2.2 **diamond-like carbon (DLC)**
amorphous carbon material containing a sufficient fraction of sp^3 hybridized carbon atoms, usually stabilized by hydrogen, to impart a high hardness

NOTE 1 In this context high hardness means greater than 20 GPa as measured according to BS EN ISO 14577-4.

*NOTE 2 This term is used in the literature and by industry to describe a wide range of carbon-based coatings, some of which do not comply with **6.2.2**.*

6.2.3 **fullerene-like carbon film**
thin films with a microstructure that resembles the structure of **fullerenes**

*NOTE The carbon atoms are arranged in sheets curved in 3-D due to the incorporation of pentagonal and heptagonal defects in the structure of **graphene**. The induced microstructure should be evident (in HREM) by the presence of swirls and closed loops. The microstructure should persist over several unit cells (10-20 nm) to clearly distinguish the **fullerene** microstructure from **amorphous carbon**. The main difference between a **fullerene**-like microstructure and **turbostratic carbon** is the presence of swirls and loops in the former while the latter mainly consists of distorted graphitic sheets.*

6.2.4 **glassy carbon (g-C)**
predominantly sp^2 bonded **amorphous carbon** containing **graphene**-like and **fullerene**-like structures

6.2.5 **tetrahedral amorphous carbon (ta-C)**
non-hydrogenated **amorphous carbon** containing over 80% sp^3 hybridized carbon

7 Fullerenes

7.1 Synthesis

7.1.1 **plasma condensation**
coalescence from a carbon plasma

7.1.2 **pulsed laser ablation (PLA)**
use of short high intensity laser pulses directed at a carbon target to generate a plume of plasma

*NOTE Condensation can occur within the plasma to produce **fullerenes**.*

7.2 Materials

7.2.1 **bridged fullerene**
fullerene where two or more nonadjacent atoms are linked by additional atoms which might be outside or inside the **fullerene** molecule.

7.2.2 buckminsterfullerene
type of **fullerene** with 60 atoms in the structure of a soccer ball (12 pentagons and 20 hexagons)

*NOTE This is the smallest **fullerene** in which no two pentagons share an edge.*

7.2.3 endohedral fullerene
fullerene with additional atoms, ions, or clusters enclosed within its shell

7.2.4 exohedral fullerene
fullerene with additional atoms, ions, or clusters attached to the outside of the **fullerene** shell

7.2.5 fullerene derivative
compound that has been formed from **fullerene** by substitution of carbon or covalent attachment of a moiety

[DD ISO/TS 80004-3:2010, definition **3.2**]

7.2.6 fullerene-doped polymer
polymer with **fullerene** molecules bonded along the backbone

7.2.7 fullerene radical ions
radical ions formed by the addition of an electron to, or removal of an electron from, a **fullerene**

7.2.8 fullerite crystal
ordered array of **fullerenes**

7.2.9 fulleroid
molecule whose structure resembles that of a **fullerene** but does not conform to the definition of a **fullerene**

NOTE Often named "modified fullerene".

[Adapted from IUPAC Recommendations for Nomenclature for the C_{60}-I_h and C_{70}-$D_{5h(6)}$ Fullerenes [2], clause Fu-1.3]

7.2.10 fused fullerene
fullerene which is incorporated into a more complex structure by sharing atoms with the surrounding molecules

[Adapted from IUPAC Recommendations for Nomenclature for the C_{60}-I_h and C_{70}-$D_{5h(6)}$ Fullerenes [2], clause Fu-7]

7.2.11 heterofullerene
fullerene that includes elements other than carbon

[Adapted from IUPAC Recommendations for Nomenclature for the C_{60}-I_h and C_{70}-$D_{5h(6)}$ Fullerenes [2], clause Fu-5]

*NOTE This is synonomous with **fullerene derivative**.*

7.2.12 homofullerene
fullerene where a carbon-carbon bond has been replaced by a methylene group

*NOTE The atoms of the **fullerene** concerned are still part of the **fullerene**.*

[Adapted from IUPAC Recommendations for Nomenclature for the C_{60}-I_h and C_{70}-$D_{5h(6)}$ Fullerenes [2], clause Fu-4.1]

7.2.13 metallofullerene
endohedral fullerene with an enclosed metal ion or ions

[DD ISO/TS 80004-3:2010, definition **3.4**]

7.2.14 norfullerene

fullerene structure from which carbon atoms have been removed

[Adapted from IUPAC Recommendations for Nomenclature for the C_{60}-I_h and C_{70}-$D_{5h(6)}$ Fullerenes [2], clause Fu-7]

NOTE The dangling bonds created are usually satisfied by hydrogen.

7.2.15 ring-fused fullerene

fullerene that shares an adjacent pair of atoms with an organic ring or ring system

[Adapted from IUPAC Recommendations for Nomenclature for the C_{60}-I_h and C_{70}-$D_{5h(6)}$ Fullerenes [2], clause Fu-7]

8 Characterization

NOTE The techniques included here are those of particular relevance to the characterization of carbon nanostructures. Other characterization techniques of general relevance to carbon nanomaterials are considered in PAS 133, Terminology for nanoscale measurement and instrumentation.

8.1 anti-Stokes scattering

scattering of light by a material where the scattered photon has higher energy than the incident photon

NOTE 1 This gives rise to an anti-Stokes line on the higher energy or shorter wavelength side of the incident spectrum.

*NOTE 2 This term is used in **Raman spectroscopy**.*

8.2 elastic recoil detection

method in which measurement of the elastic scattering of ions is used to analyse for light elements in a solid

NOTE For carbon materials, the method is often used to determine the hydrogen content, for example, in a-C:H.

8.3 electron energy loss spectroscopy (EELS)

method in which the energy distribution spectrum of electrons inelastically scattered as they pass through a material is used to determine compositional and structural information about the material

NOTE For carbon materials, it is a well established method for probing the existence of sp^2 and sp^3 hybridized atoms.

8.4 Fourier transform infrared spectroscopy (FTIR)

analytical chemical technique, based on spectroscopy, in which a gaseous sample is subjected to excitation of molecular bonds by pulsed, broad-band infrared radiation, and the Fourier transform mathematical method is used to obtain an absorption spectrum

[BS EN ISO 13943:2010, definition **4.158**]

NOTE Used to probe bonding types and structures, e.g., double and triple carbon-carbon bonds, and bonds with other elements, such as hydrogen, nitrogen, oxygen, present in a carbon material.

8.5 near edge X-ray absorption fine structure (NEXAFS)
characterization using measurement of the energies of photons and electrons emitted from matter following irradiation with photons of energies close to the absorption edge of the material, to derive structural information about the irradiated material

NOTE 1 This can provide valuable information about bonding in molecular structures.

NOTE 2 Requires an intense tunable source of soft X-rays, hence undertaken at synchrotrons.

8.6 photoconductivity
increase in conductivity of a material when illuminated with light

NOTE Gives information on transport and recombination processes for carbon materials.

8.7 photoluminescence (PL)
luminescence caused by absorption of optical radiation

[IEC 60050-845:1987,04-19]

NOTE Gives information on the recombination process of electrons and holes and, for carbon materials, it is attributed to the recombination of electron-hole pairs confined in π-rich entities surrounded by a sp^3 matrix.

8.8 radial breathing mode (RBM)
strongest low frequency Raman mode for **carbon nanotubes**

NOTE Commonly used to determine the diameter of ***carbon nanotubes****.*

8.9 Raman effect

emitted radiation, associated with molecules illuminated with monochromatic radiation, characterized by an energy loss or gain arising from rotational or vibrational excitations

[BS ISO 18115-2:2010, **6.128**]

NOTE Hence, this changes the energy of the scattered photon.

8.10 Raman D-peak

peak in the Raman spectrum of carbon-containing materials at about 1350 cm^{-1} for optical wavelength excitation

NOTE Directly linked to the breathing mode of aromatic carbon rings and used as an indication of disorder.

8.11 Raman G-peak

peak in the Raman spectrum of carbon-containing materials at about 1590 cm^{-1} for optical wavelength excitation

*NOTE Directly linked to sp^2 bonded carbon and used as an indication of ordering. Many researchers use the I(D)/I(G) ratio of the intensities of the G and D peaks to assess the amount of disorder in carbon films.*3)

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3) Chem. Phys., 2007, **9**, 1276-1290; DOI: 10.1039/b613962k.

8.12 Raman spectroscopy

spectroscopy in which the **Raman effect** is used to investigate molecular energy levels

[Adapted from BS ISO 18115-2:2010, **6.129**]

8.13 Rutherford back scattering (RBS)

method in which the scattering of high energy ions is used to determine compositional and structural information about a solid

NOTE The technique can be used, for example, to determine the variation of sp^3 *fraction and the density of a carbon film.*

8.14 small angle X-ray scattering (SAXS)

method in which analysis of the scattering of X-rays at angles close to the transmitted beam is used to determine structural information about materials

NOTE This method can be used to obtain data on ultrananocrystalline diamond nucleation and growth behind the ***detonation*** *wavefront.*

8.15 Stokes scattering

scattering of light by a material where the material absorbs energy and the scattered photon has a lower energy

NOTE 1 This gives rise to a Stokes line on the lower energy or longer wavelength side of the incident spectrum.

NOTE 2 This term is used in ***Raman spectroscopy****.*

8.16 synchrotron radiation small angle X-ray scattering (SRSAXS)

<as **8.14**> where synchrotron radiation is used as the source of X-rays

NOTE 1 Synchrotron radiation produces a beam with much higher intensity than conventional X-ray sources, allowing much shorter exposure times to be used.

NOTE 2 This method can be used to elucidate aspects of the ultrananocrystalline diamond formation kinetics.

8.17 thermogravimetric analysis (TGA)

chemical analysis by the measurement of weight changes of a system or compound as a function of increasing temperature

[McGraw-Hill Dictionary of Scientific and Technical Terms, 6th edition, published by The McGraw-Hill Companies, Inc]

8.18 X-ray Auger electron spectroscopy (XAES)

method in which an electron spectrometer is used to measure the energy distribution of Auger electrons emitted from a surface after irradiation with X-rays

NOTE 1 This method is extensively used to determine the bond angles and nearest neighbour atom distance in carbon films. ***NEXAFS XAES*** *data has been used to determine* ***carbon hybridization****, and the detection of diamond-like bonding in a-C films.*

NOTE 2 Requires an intense tunable source of soft X-rays, hence undertaken at synchrotrons.

8.19 X-ray photoelectron spectroscopy (XPS)

method in which an electron spectrometer is used to measure the energy distribution of photoelectrons and Auger electrons emitted from a surface irradiated by X-ray photons

NOTE 1 X-ray sources in common use are unmonochromated Al Kα and Mg Kα X-rays at 1 486.6 eV and 1 253.6 eV, respectively. Modern instruments also use monochromated Al Kα X-rays. Some instruments make use of various X-ray sources with other anodes or of synchrotron radiation.

[BS ISO 18115-1:2010, **4.23**]

NOTE 2 This method has been used to measure ***carbon hybridization*** *at the surface of carbon materials such as diamond,* ***amorphous carbon*** *and* ***DLC****.*

Annex A (informative)

Abbreviations

a-C	Amorphous Carbon
a-C:H	Amorphous Hydrogenated carbon
CNT	Carbon Nanotube
CVD	Chemical Vapour Deposition
CVS	Chemical Vapour Synthesis
DLC	Diamond-Like Carbon
DWCNT	Double-wall Carbon Nanotube
ECR	Electron Cyclotron Resonance
ECWR	Electron Cyclotron Wave Resonance
EELS	Electron Energy Loss Spectroscopy
FCVA	Filtered Cathodic Vacuum Arc
FTIR	Fourier Transform Infrared Spectroscopy
g-C	Glassy Carbon
HFCVD	Hot Filament Chemical Vapour Deposition
HPHT	High Pressure High Temperature
MWCNT	Multiwall Carbon Nanotube
NEXAFS	Near Edge X-ray Absorption Fine Structure
PECVD	Plasma Enhanced Chemical Vapour Deposition
PL	Photoluminescence
PLA	Pulsed Laser Ablation
PVD	Physical Vapour Deposition
PVS	Physical Vapour Synthesis
RBM	Radial Breathing Mode
RBS	Rutherford Back Scattering
SAXS	Small Angle X-ray Scattering
SRSAXS	Synchrotron Radiation Small Angle X-ray Scattering
SWCNT	Single-wall Carbon Nanotube
ta-C	Tetrahedral Amorphous Carbon
TGA	Thermogravimetric Analysis
UDD	Ultradispersed Diamond
XAES	X-ray Auger Electron Spectroscopy
XPS	X-ray Photoelectron Spectroscopy

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4) Available at www.chem.qmul.ac.uk/iupac/fullerene/

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