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PUBLICLY AVAILABLE SPECIFICATION

PRE-STANDARD

colour inside

Nanomanufacturing – Material specifications – Part 2-1: Single-wall carbon nanotubes – Blank detail specification

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FOREWORD

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IEC-PAS 62565-2-1 has been processed by IEC technical committee 113: Nanotechnology standardization for electrical and electronic products and systems.

The text of this PAS is based on the following document:	This PAS was approved for publication by the P-members of the committee concerned as indicated in the following document
Draft PAS	**Report on voting**
113/100/PAS	113/105A/RVD

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INTRODUCTION

This Publicly Available Specification is intended to provide guidance on how to list, illustrate and define various characteristics of single-wall carbon nanotubes (SWCNTs) for industrial use in electronic products, and how to incorporate these into a bilateral detail specification between vendor and user.

One particular point of interest is the fact that there are different modifications of carbon nanotubes. Subtle differences in the physical structure lead to marked differences in electrical, optical and chemical properties; therefore these characteristics need special attention.

To permit common processing equipment and common unit processes with predictable and reproducible results to be used in multiple fabrication lines, it is essential for the carbon nanotubes characteristics to be described and assessed in a standardized manner and to standardize the methods for quality control of the manufacturing processes.

To enable low-cost mass production (or production of pure fractions), a reliable, affordable means of preparing one type of carbon nanotubes (e.g. single-wall semiconducting carbon nanotubes, with a certain specified length) is necessary. To facilitate a reliable source of carbon nanotubes with tailored properties (length, diameter, purity, chirality, conduction type), it is necessary to specify the characteristics in a standardized way, stating the specification limits and the characterization methods to prove conformance. This does not only reduce transaction costs, but eliminates a major source of error, as explained below.

Accurately measuring and characterising the quality of nanotube-containing materials and the dispersion of nanotubes in liquids or polymers, are both considered crucial for the continued growth of applications incorporating single-wall carbon nanotubes. Significant differences in both methodology and interpretation continue to exist from one measurement laboratory to another. For this reason, comparison and specification of the quality of CNT materials is extremely difficult. While progress in these measurements is being been made, significant improvements are still needed to accurately measure and characterise the quality of carbon nanotube-containing materials and the protocol for doing so (e.g. how to describe / specify the characteristics relevant for the quality of the final nano-enabled product).

Furthermore, the development of reference materials is as important as improvements to measurement / characterization techniques. In addition, it is stressed that for any of the analysis methods, it is mandatory to specify the sample preparation method, sample size and the sampling method.

Experiences with this PAS should be reported to the Secretariat of IEC Technical Committee 113 to provide improvements for the future IEC 62565 International Standards under development in IEC/TC 113.

NANOMANUFACTURING – MATERIAL SPECIFICATIONS –

Part 2-1: Single-wall carbon nanotubes – Blank detail specification

1 Scope

This PAS establishes a blank detail specification for the essential electrical properties and certain other common characteristics including dimensional, structural and mechanical properties of single-wall carbon nanotubes.

This PAS provides a standardized format for detail specifications characterising essential basic properties of single-wall nanotubes and recommends measurement methods.

Single-wall carbon nanotubes with a chemical modification, dispersed into a solvent or grown on a substrate are included.

Properties and characteristics not of relevance for a specific application may be classified as not applicable or not specified.

NOTE 1 The present state of the art in manufacturing carbon nanotubes does not produce purely single-wall carbon nanotubes. The consequences are reflected in the requirements part.

NOTE 2 A revisable version of Tables 2 to 8 is attached to this file. These tables are intended to be used in the detail specification to be agreed between manufacturer and user of single-wall carbon nanotubes.

Microsoft Word Document

2 Normative references

The following referenced documents are indispensable for the application of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

IEC 62624, *Test methods for measurement of electrical properties of carbon nanotubes*

NOTE 1 Supplementary information is provided in the bibliography

NOTE 2 Terminology and nomenclature are under development in IEC/TC113/JWG 1 in cooperation with ISO/TC 229. Published terminology standards or specifications from this group will be incorporated into this document.

NOTE 3 Measurement and characterization are under development in IEC/TC113/JWG 2 in cooperation with ISO/TC 229. Published measurement standards or specifications from this group will be incorporated into this document.

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

NOTE 1 Terminology and nomenclature are under development in IEC/TC113/JWG 1 in cooperation with ISO/TC 229. Published definitions from this group will be incorporated into this document. Not yet specified definitions are taken from the scientific literature.

NOTE 2 Measurement and characterization are under development in IEC/TC113/JWG 2 in cooperation with ISO/TC 229. Published definitions from this group will be incorporated into this document. Not yet specified measurement methods are taken from the scientific literature.

3.1
chirality

twist of carbon nanotubes, determined by the values of n and m for the chiral vector $\vec{C}_h$ according Figure 1

NOTE Chirality affects the conductance of the nanotube, density, lattice structure, and other properties. The chiral vector is defined in Table 1 in terms of the integers (n, m) and the basis vectors of the lattice, which are given in terms of rectangular coordinates.

3.2
diameter of single-wall carbon nanotubes

d_t

diameter uniquely determined by the integers (n, m)

3.3 Acronyms and abbreviations

AFM	Atomic Force Microscopy
BET	Brunauer-Emmett-Teller method to determine the surface area by gas absorption [2] [1)]
CNT	Carbon Nanotube
CVD	Chemical Vapour Deposition
EDX	Energy Dispersive X-Ray Fluorescence Spectrometry
EFM	Electrostatic Force Microscopy
GPC	Gel Permeation Chromatography
HPLC	High Performance Liquid Chromatography
ICP-MS	Inductively Coupled Plasma - Mass Spectrometry
NIR	Near Infrared Spectroscopy
PL	Photoluminescence
Raman	Raman Spectroscopy
SWCNT	Single-wall Carbon Nanotube
MWCNT	Multiwall Carbon Nanotube
SEM	Scanning Electron Microscopy
SGM	Scanning Gate Microscopy
SPM	Scanning Probe Microscopy
SPS	Surface Photo Voltage Spectroscopy
STS	Scanning Tunnelling Spectroscopy
SThPM	Scanned Thermal Probe Microscopy

1) Numerals in square brackets refer to the Bibliography.

STM	Scanning Tunnelling Microscopy
TGA	Thermogravimetric Analysis
TG-MS	Thermogravimetry–Mass Spectrometry
TEM	Transmission Electron Microscopy
UV	Ultraviolet Spectroscopy
UV-vis-NIR	UV-vis-NIR Absorption Spectroscopy
XPM	X-ray Photoelectron Microscopy
XPS	X-ray Photoelectron Spectroscopy

4 Basic information

This clause summarizes the fundamental characteristics for single-wall carbon nanotubes, gives the basic relations governing these parameters and lists typical numeric values for these parameters.

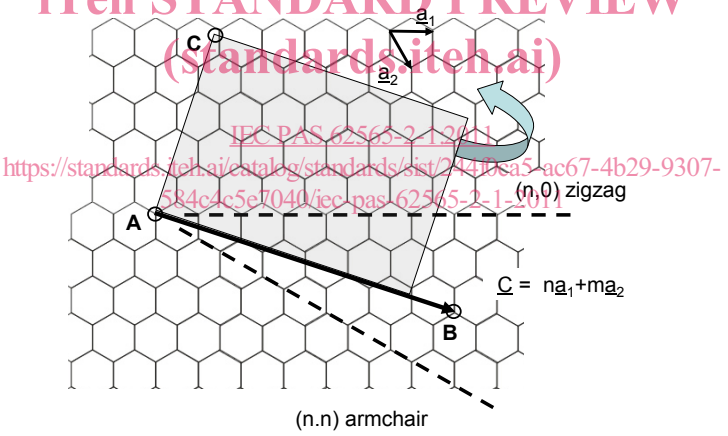

Figure 1 – Two-dimensional graphene sheet with vectors defining chirality

In single carbon layers of graphite each carbon atom is bound to three neighbours in a honeycomb structure. The chiral vector C_h is the connection between the points A and B, which coincide when the gray area is rolled up to form a short section of a carbon nanotube. The axis of the tube is parallel to the line AC. For the special case $n = m$ (as defined in Figure 1 and Table 1) the **armchair configuration** results, and for $m = 0$ the **zig zag configuration** results, see Figure 2 and Figure 3. Depending on the values of n and m the carbon nanotube is either semiconducting or metallic. The angle between the vector a_1 and the chiral vector C_h is defined as the chiral angle Θ. The length of chiral vector L is directly related to the tube diameter.

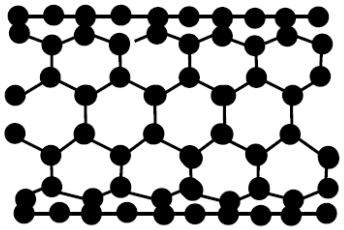

Figure 2 – Example of armchair tube (θ = 30° direction, θ as defined in Table 1)
(view perpendicular to the CNT axis)

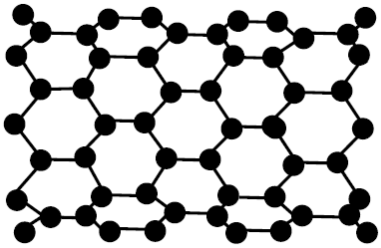

Figure 3 – Example of zigzag tube (θ = 0° direction, θ as defined in Table 1),
(view perpendicular to the CNT axis)

Table 1 – Parameters of single-wall carbon nanotubes [1]

Symbol	Name	Formula	Value
$a_{C\text{-}C}$	Carbon-Carbon distance sp^2		0,1421 nm for graphene
A	Length of unit vector	$\sqrt{3}a_{C-C}$	in (x, y) coordinates
$\underline{a}_1, \underline{a}_2$	Unit vectors	$\left(\sqrt{3}/2, \frac{1}{2}\right)a, \left(\sqrt{3}/2, -\frac{1}{2}\right)a$	in (x, y) coordinates
$\underline{C}_h$	Chiral vector	$n \cdot \underline{a}_1 + m \cdot \underline{a}_2 \equiv (n, m)$	n, m: integers
L	Circumference of nanotube	$a\sqrt{n^2 + m^2 + nm} = \lvert\underline{C}_h\rvert$	$0 \le \lvert m \rvert \le n$
d_t	Diameter of nanotube	$\frac{L}{\pi}$	
Θ	Chiral angle (inner wall)	$\tan\theta = \frac{\sqrt{3}m}{2n + m}$	$0 \le \lvert\theta\rvert \le 30°$

5 General introduction regarding measurement methods

The specification of material parameters of carbon nanotubes has to refer to measurement methods for which currently no standards exist. Standardized methods for the characterization of carbon nanotubes are under development. For reasons of practicality for industrial use in manufacturing of electronic products, this PAS recommends only one measurement method for each material parameter.