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The weight and density of carbon nanotubes versus the number of walls and diameter

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ABSTRACT

The weight and density of carbon nanotubes are calculated as a function of their characteristics (inner diameter, outer diameter, and number of walls). The results are reported in the form of diagrams which may be useful to other researchers, in particular in the fields of synthesis/production, materials and composites, health/toxicity studies.

In the early years of research on carbon nanotubes (CNTs), many conflicting results have been reported, mainly because the authors did not use the same CNTs and CNT samples. It was later fully recognized that several kinds of

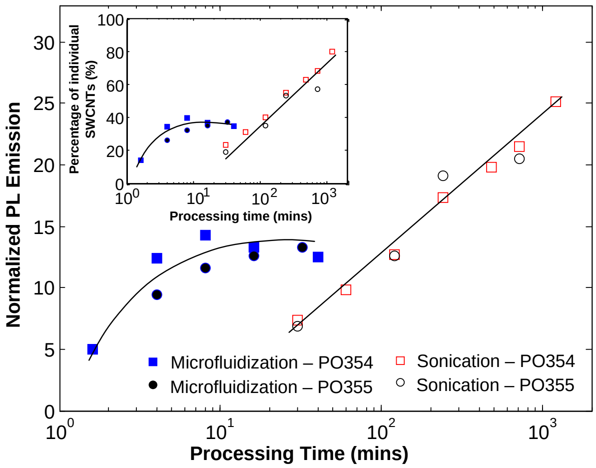

Fig. 3 – Effects of ultrasonication and microfluidization processes on the G-band normalized photoluminescence and the degree of separation of dispersions into individual SWCNTs. Solid lines are for guidance only.

separating the SWCNT bundles into individual tubes. A wise design of the micro-mixing chamber with consideration of the flow field effect should be considered in the future for improving the microfluidization process as a useful technique in producing high quality SWCNT dispersions.

In summary, a comparison of two distinct SWCNT processing techniques – the microfluidization versus the ultrasonication process has been made. Despite its inefficiency in energy utilization and separation of SWCNT bundles, the microfluidization process, as facilitated by the extremely high energy dissipation rate, is a useful technique for the high throughput and large-scale production of SWCNT dispersions. More importantly, the types of flow field rather than the energy dissipation rate have been identified as a critical factor in separating the SWCNT bundles into individual tubes.

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CNTs do exist, such as single-walled CNTs (SWCNTs), double-walled CNTs (DWCNTs) and multi-walled CNTs (MWCNTs). Note that some confusion remains because hollow carbon nanofibers that do not show the particular continuous concentrical structure are sometimes noted CNTs or MWCNTs. It was also taken into account that the different synthesis routes produce CNTs with different lengths, crystallinity and defect proportion and CNT samples with different levels of purities (carbon element versus other elements and CNTs versus other carbon species). However, the fact that a SWCNT and a MWCNT of the same length do not have the same weight has been neglected until now. Indeed, companies use gross carbon tonnages as CNT production figures, and research works, for example on CNT-composite materials, generally use the term "CNT content" when in fact "carbon content" should be used. In this work, we report calculations establishing the relations between the weight and the density of CNTs and their geometrical characteristics (inner diameter, outer diameter, and number of walls). The results are reported in the form of diagrams which may be useful to other researchers, in particular in the fields of synthesis/production, materials and composites and also health/toxicity studies, where the number of CNTs in a given sample is extremely more relevant than the weight itself.

The calculations are based on the following hypotheses: (i) the length of the C=C bonds in the curved graphene sheets is the same than in the planar sheet i.e. $d_{C=C} = 0.1421$ nm, (ii) the MWCNTs are composed of concentric shells (inter-shell distance $d_{s-s} = 0.3400$ nm), (iii) the contribution of the electron density to the outer diameter is neglected and (iv) the aspect ratio of CNTs is sufficiently high (>1000) to neglect the area of the tip surfaces in comparison to the area of the cylindrical surfaces. As reported earlier [1], the specific surface area of a SWCNT, whatever its diameter, is that of one side of a graphene sheet, i.e. 1315 m^2/g. Thus, the weight of any SWCNT (W_{SW}) of diameter d and length L can be calculated from the surface area of the graphene sheet:

$$W_{SW} = \frac{1}{1315}\pi L d \text{ (grams)} \qquad (1)$$

We now consider a MWCNT with an inner diameter d_{int}, the same length L and a number of walls n. The surface area of all the graphene sheets which compose the MWCNT is:

$$S_{MW} = \pi \cdot L \cdot \{d_{int} + (d_{int} + 2 \cdot d_{s-s}) + (d_{int} + 4 \cdot d_{s-s}) + \cdots + [d_{int} + 2(n-1) \cdot d_{s-s}]\} \qquad (2)$$

which can be simplified:

$$S_{MW} = \pi L \left[n d_{int} + 2 d_{s-s} \sum_{i=0}^{n-1} i \right] \qquad (3)$$

Each graphene sheet has a surfacic weight equal to 1/1315 g/m^2 and thus the weight of the MWCNT (n walls, length L) (w_{MW}) can be calculated:

$$W_{MW} = \frac{1}{1315} \cdot \pi L \left[n d_{int} + 2 d_{s-s} \sum_{i=0}^{n-1} i \right] \qquad (4)$$

In order to simplify the comparison, taking the same length for the two CNTs, the weight of the MWCNT (w_{MW}) of inner diameter d_{int} (Eq. (4)) is divided by the weight of the SWCNT (Eq. (1)), 1 nm in diameter, giving the ratio R:

$$R = w_{MW}/w_{(SW,1\,nm)} = \left[n d_{int} + 2 d_{s-s} \sum_{i=0}^{n-1} i \right] \quad \text{with } d_{int} \text{ in nm} \qquad (5)$$

The volume of one CNT depends on the outer diameter (d_{out}):

$$V_{MW} = \pi L d_{out}^2 / 4 \qquad (6)$$

and the weight of the CNT is given by Eq. (4), transformed as a function of d_{out} as opposed to d_{int}:

$$W_{MW} = \frac{1}{1315} \cdot \pi L \left[n d_{out} - 2 d_{s-s} \sum_{i=0}^{n-1} i \right] \qquad (7)$$

The density (d_{MW}) of a MWCNTs is thus:

$$d_{MW} = 1000 \cdot w_{MW}/V_{MW} = \frac{4000}{1315} \left[n/d_{out} - \left(2 d_{s-s} \sum_{i=0}^{n-1} i \right) / d_{out}^2 \right] \quad \text{with } d_{out} \text{ in nm} \qquad (8)$$

R was plotted versus the number of walls n, for different values of d_{int} (Fig. 1) and the density was plotted versus d_{out} for different number of walls (Fig. 2).

For a SWCNT, 1 nm in diameter, $R = 1.00$. Simply adding one wall, i.e. considering a DWCNT with $d_{int} = 1$ nm (solid circle in Fig. 1), results in a strong increase of R (2.68). For a MWCNT with 10 walls and $d_{int} = 5$ nm (open circle in Fig. 1), $R = 80.60$. Thus, the production of 1 ton of (SWCNTs, 1 nm) is equivalent, in terms of the number of CNTs of same length, to the production of 2.68 tons of (DWCNTs, $d_{int} = 1$ nm) and 80.60 tons of (MWCNTs, 10 walls, $d_{int} = 5$ nm). If one takes into

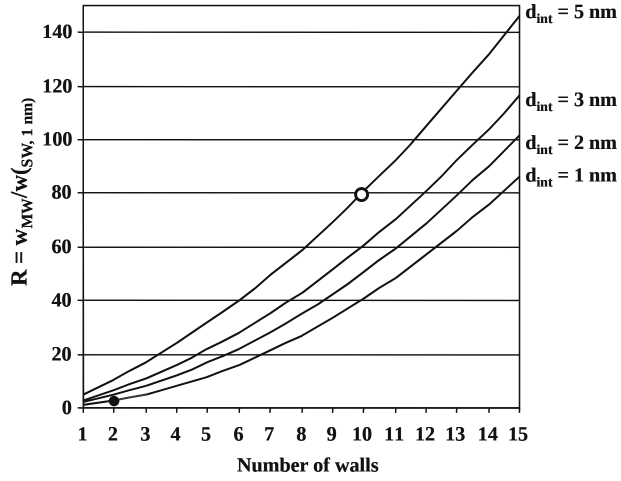

Fig. 1 – The ratio R of the weight of a MWCNT of inner diameter d_{int} and length L to the weight of a SWCNT of diameter 1 nm and length L versus the number of walls n, for different values of d_{int}.

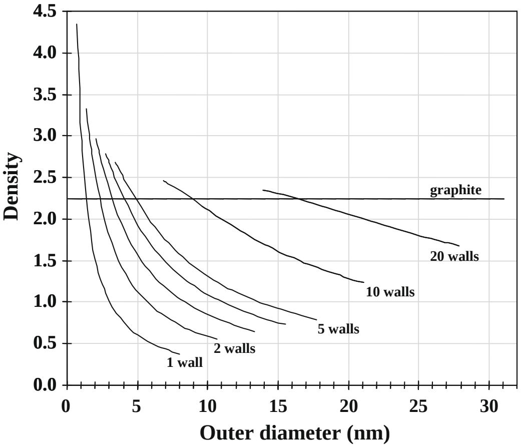

Fig. 2 – The density (d_{MW}) of CNTs versus the outer diameter for different number of walls.

account that the typical length of MWCNTs and SWCNTS is about 100 and 10 μm, respectively, there would be a factor of *ca.* 800 between the respective weight of samples containing the same number of CNTs. The density (Fig. 2) increases dramatically when decreasing the diameter, in particular for SWCNTs and DWCNTs. For example, the density of a SWCNT, $d_{out} = 3$ nm, is equal to 1, whereas it is equal to 1.8 for a DWCNT, $d_{out} = 3$ nm. Below a certain diameter, the density is higher than that of graphite. Although this could be counter-intuitive, it reflects the fact that a CNT is a 1D object whereas graphite is 2D, with an absence of matter on the lateral sides. Note also that the density is lower by a few percent if the CNTs are forming organized bundles, which is not taken into account here. Therefore, it is clear that the carbon content in a composite material or test sample cannot be translated into the CNTs content without a precise knowledge of the geometry of the CNTs in question.

Johnson et al. [2] have mentioned that the density of their MWCNTs is 1.1 as calculated from the microscopic structure. Our calculation from their data (outer diameter 70 nm, 30 walls) give 1.12, which is in excellent agreement. Zhan et al. [3] have indeed mentioned that the density of CNTs is a function of both their diameter and their number of shells, but these authors give no example. The estimated density for their SWCNTs is 1.8. We have measured by He pycnometry the apparent density of one of our samples, consisting mainly of DWCNTs, with also SWCNTs and CNTs with three walls [4]. The obtained value is in the range 1.86–1.94 which is in broad agreement with the expected value of 1.92 calculated using the hypothesis that the sample contains only carbon (92 wt.%) and cobalt (8 wt.%, which is overestimated). Note that since the specific surface area of this sample is equal to 923 m^2/g, applying a proper outgassing procedure is very important. Kim et al. [5] have reported that the measured density is equal to 1.74 ± 0.16 for two different samples of CNTs (outer diameters about 15 nm and about 22 nm). No experimental details are given on the number of walls other than “a diameter of 15 nm corresponds to about 20 graphite layers”. Our calculations from their data give the following results for the two samples: (15 nm, 11 walls, 1725) and (22 nm, 17 walls, 1769). Given that their measured density range is 1.58–1.90, this represents a good agreement.

In conclusion, it is shown that both the weight and density of CNTs vary over a very wide range depending on the number of walls, inner diameter or outer diameter. The results are reported in the form of diagrams which may be useful to other researchers, in particular in all areas where carbon content and CNT content should not be confused.

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