

Supplementary Information

Shear force mixing versus ultrasonication of solution-processing carbon nanotubes for field-effect transistor applications

(Journal of Materials Science: Materials in Electronics)

Debjani Goswami, Petro Lutsyk

Aston Institute of Photonic Technologies, School of Engineering and Innovation, Aston University, Aston Triangle, B4 7ET, Birmingham, UK

Corresponding author e-mails: d.goswami@aston.ac.uk (D.G.), p.lutsyk@aston.ac.uk (P.L.)

S1. Gaussian fitting of absorption and PL spectra

Absorption spectra of small diameter SWNTs have been fitted by Gaussian curves in the range of 900-1100nm (or ca. 1.14-1.36 eV; the eV range is more appropriate for Gaussian fittings). The first iteration of such fitting was to consider the peaks of (6,5) and (7,5) chiralities by two Gaussians around 1.206 eV and 1.24 eV and third Gaussian around higher-energy peak 1.325-1.33 eV. This three-Gaussians fitting is shown in Figure S1a,b, evidencing a fitting gap of in the range of 1.25-1.30 eV, thus requiring use of one more Gaussian curve in this range. Therefore, in Figure S1c,d, four-Gaussians fittings are presented with extra peak at 1.267 eV added. Higher energy peaks can feature other chiralities present, for example (7,0) and/or (6,2) [SI-1]. Table S1 summarizes key parameters of above Gaussian fittings. The following formula (S1) for the Gaussian function was used [SI-2]:

$$f(x) = Ae^{-\frac{(x-x_0)^2}{2\sigma^2}} \quad (S1)$$

where A is the amplitude of the peak, x_0 is peak position {in eV}, σ denotes the standard deviation and corresponds to the half-width of the Gaussian curve at the half-maximum {in eV}, i.e. representing half-width at half-maximum (HWHM) of the E_{11} peaks.

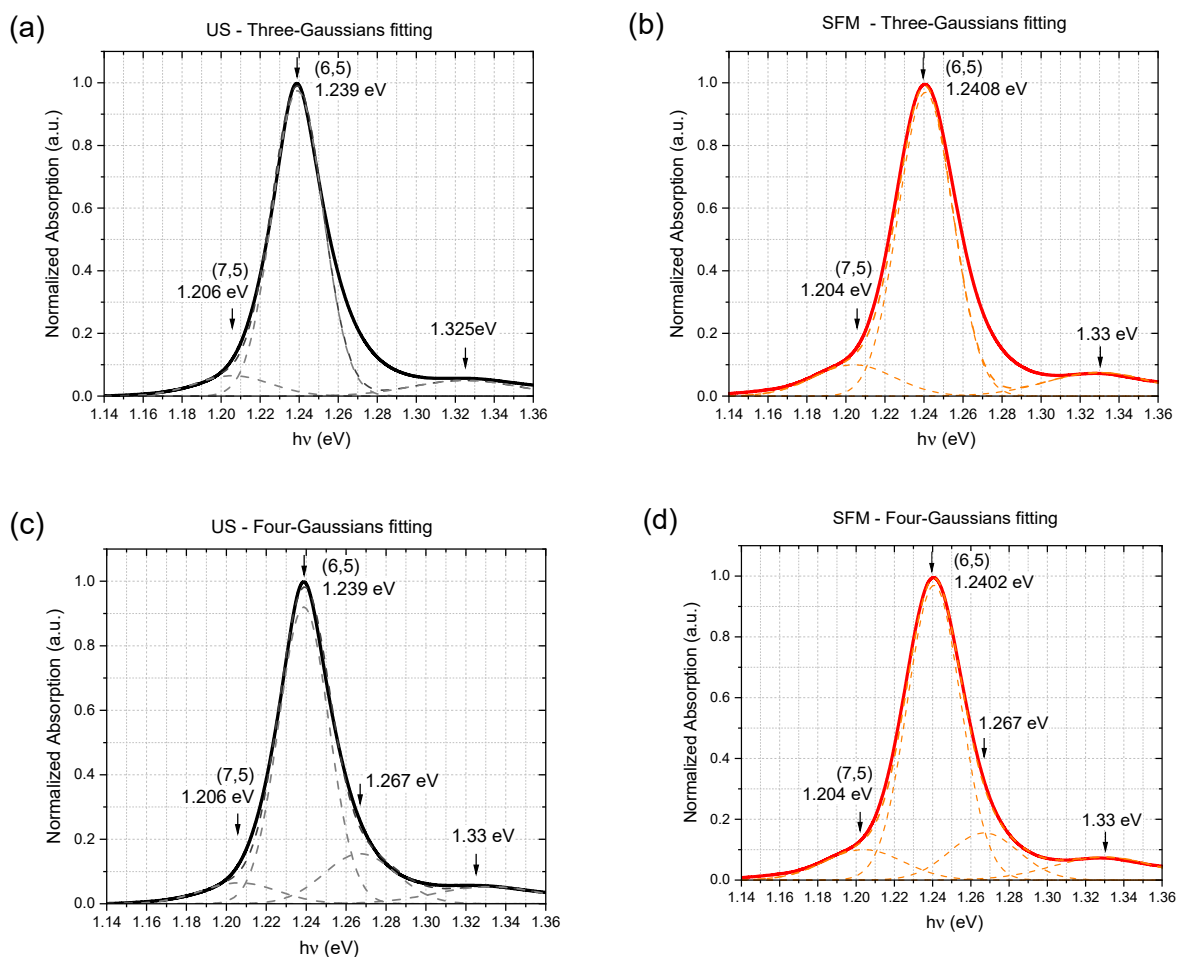


Fig. S1 Normalized absorption spectra of small diameter SWNT dispersed by US (a,c) and SFM (b,d) supplemented with their three- (a,b) and four-Gaussians (c,d) fitting

Table S1. Parameters of three-Gaussians fitting shown in Figure S1a,b and four-Gaussian fitting shown in Figure S1c,d using equation S1

Three-Gaussians fitting												
	Band 1			Band 2						Band 3		
	A	x ₀	σ	A	x ₀	σ				A	x ₀	σ
US	0.065	1.206	0.019	0.98	1.239	0.013				0.05	1.33	0.027
SFM	0.100	1.204	0.021	0.97	1.241	0.014				0.075	1.33	0.027
Four-Gaussians fitting												
	Band 1			Band 2			Band 3			Band 4		
	A	x ₀	σ	A	x ₀	σ	A	x ₀	σ	A	x ₀	σ
US	0.065	1.207	0.019	0.92	1.239	0.013	0.155	1.267	0.018	0.053	1.33	0.027
SFM	0.100	1.204	0.021	0.92	1.240	0.014	0.155	1.267	0.018	0.075	1.33	0.027

PL spectra of small diameter SWNTs have been fitted by Gaussian curves in the range of 1.1-1.3 eV (Figure S2). The parameters of E_{11} PL emission peaks of the small diameter nanotubes (Table S2) can be analysed for both dispersion methods in conjunction with parameters of E_{11} absorption peaks (Table S1).

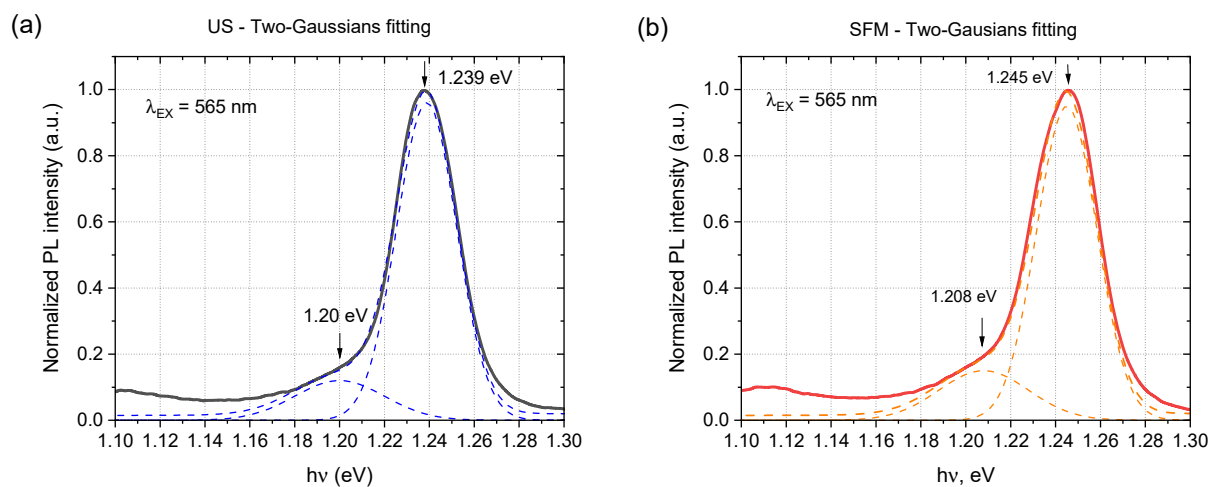


Fig. S2 Normalized PL spectra of small diameter SWNT dispersed by US (a) and SFM (b) supplemented with Two-Gaussians fitting

Table S2. Parameters of Two-Gaussians fitting shown in Figure S2 using equation S1

	Band 1			Band 2		
	A	x_0	σ	A	x_0	σ
US	0.12	1.200	0.02	0.96	1.239	0.013
SFM	0.15	1.208	0.02	0.95	1.245	0.013

In Figure S2, the HWHM values are 0.016 eV for the US dispersion and 0.017 eV nm for the SFM dispersion. Although the SFM peak is slightly broader, the Gaussian fittings produce same $\sigma = 0.013$ eV for Band 2 at 1.239-1.245 eV, therefore small difference in the HWHM might be attributed to higher contribution of Band 1 belonging to (7,5) chirality. The (7,5) chirality nanotubes emit around 1030 nm (1.2 eV), which is relatively close to the (6,5) E_{11} peak. The emissions from these two chiralities overlap and make bands broader on one side of the spectrum (without evident bends or other features of the spectra).

HWHM parameters of Gaussian fittings for absorption spectra summarized in Table S1. HWHM (σ) of Band 1 (1.204-1.207 eV) associated with (7,5) chirality is larger for SFM nanotubes; Band 2 (1.240-1.241 eV) attributed to the (6,5) chiralities have only slightly larger HWHM for SFM, whereas HWHM of Band 3,4 are same (Table S1). Considering both absorption and PL, HWHM for Band 1 absorption should be considered as more accurate due to the fitting of spectrum edge, whereas the PL spectra have additional emission in the same range. Therefore, the peaks of SWNTs of (7,5) chirality are a bit broader in SFM processed samples. HWHM for Band 2 (SWNTs of (6,5) chirality) can be considered as practically the same for both dispersion methods (the differences in σ absorption Gaussian fittings are minimal and in the range of the wavelength accuracy for a Lambda 1050 in NIR range (+/- 0.3 nm)).

S2. Additional EPL maps

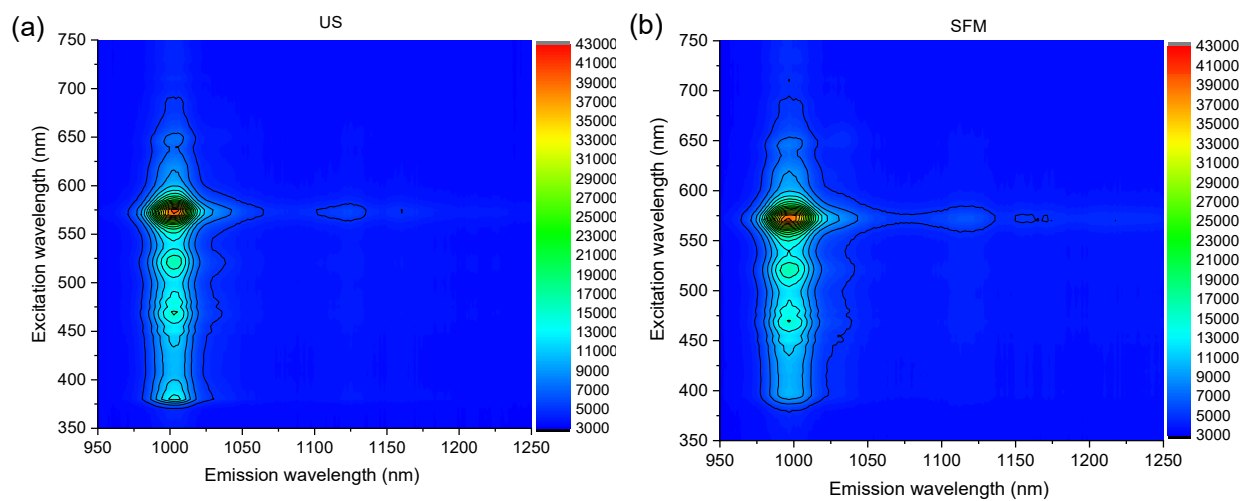


Fig. S3 EPL maps of small diameter SWNTs dispersed by US (a) and SFM (b)

S3. Lorentzian fitting for Raman Spectra in the range of G-band

The following function, $L(x)$, has been utilized for Lorentzian fitting of Raman Spectra in the range of G-band [SI-3]

$$L(x) = \frac{a}{((x-x_l)^2+b^2)} \quad (S2)$$

where x_l is the center or peak position {in cm^{-1} }, b is the half-width at half-maximum (HWHM), which determines the width of the peak (the full width at half maximum, FWHM is $2 \cdot b$) {in cm^{-1} }, and a is the product for amplitude (or peak height) and b^2 . Therefore, the amplitude (or Lorentzian peak height) is $Amp = a / b^2$:

$$L(x) = Amp \frac{b^2}{((x-x_l)^2+b^2)} \quad (S3)$$

This way, the $L(x)$ is equal to Amp at $x = x_l$. The Lorentzian fittings for Raman spectra are shown on Figure S4. Spectra of small and large diameter SWNTs were fitted with two and three Lorentzian functions, respectively (Table S3).

Table S3. Lorentzian fitting parameters for normalized Raman spectra in Figure 4 and Figure S4

	Band 1			Band 2 (G^+)			Band 3		
	a	x_l	b	a	x_l	b	a	x_l	b
small diameter; US	-	-	-	89	1594.0	9.7	14	1611.0	6.5
small diameter; SFM	-	-	-	78	1591.7	9.1	30	1612.8	6.9
large diameter; US	24	1574.0	8.5	50	1598.0	7.5	24	1611.0	8.6
large diameter; SFM	4.8	1573.0	6	55	1595.0	7.5	14	1613.7	5.7

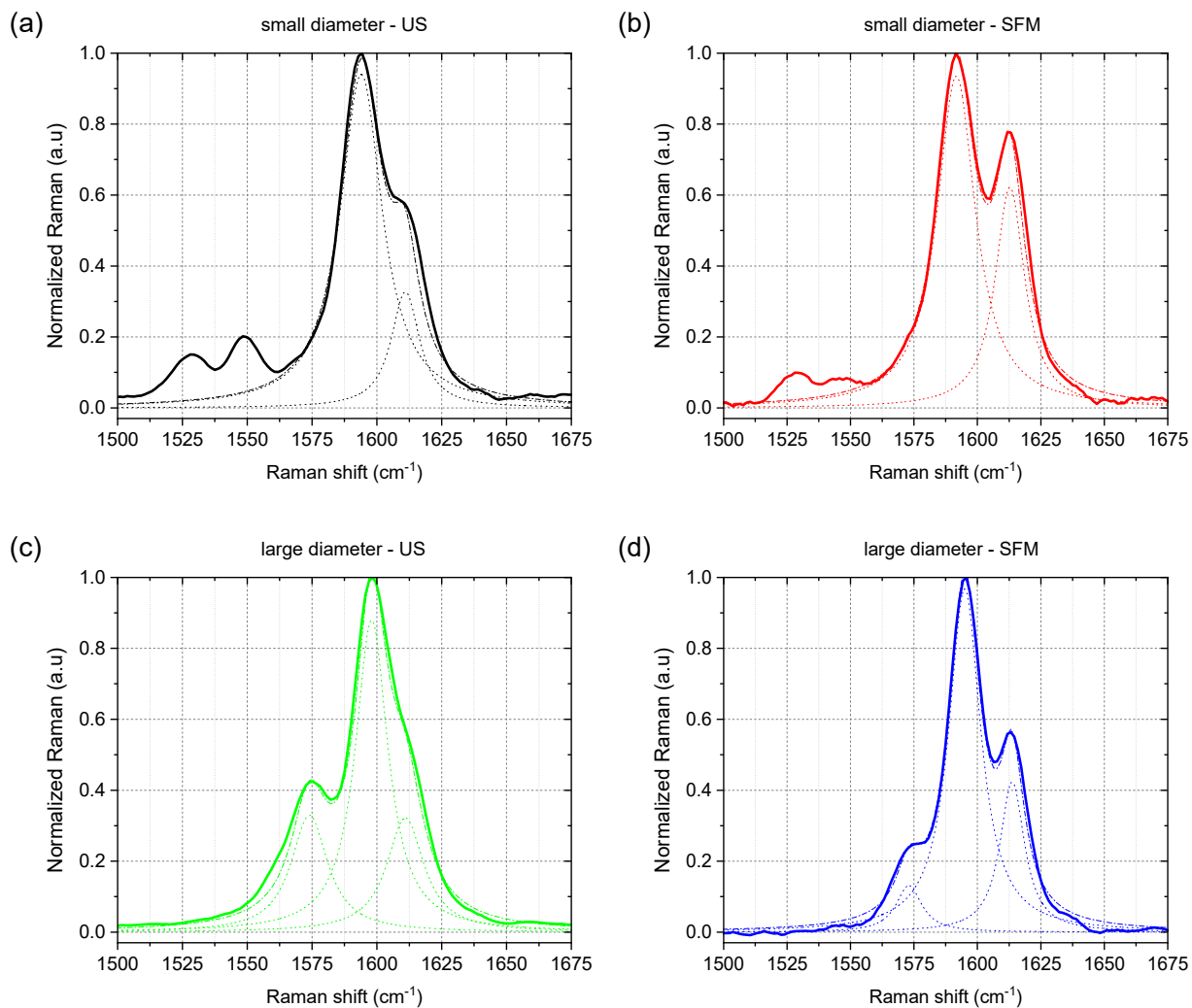


Fig. S4 Raman spectra of small (a,b) and large diameter (c,d) SWNT dispersed by US (a,c) and SFM (b,d) supplemented by Lorentzian fitting with two (a,b) and three (c,d) bands (mentioned as Band 1, 2(G^+), 3 in Table S3

Table S4. Parameters of Lorentzian fitting curves for Band 2 (G^+) using data from Table S3, intensities of 2D peak from Figure 4 and the ratio of $2D/G^+ \text{ Amp}$

	Band 2 (G^+)			2D peak (intensity)	$2D/G^+ \text{ Amp} = 2D/(a/b^2)$ (intensity)
	a	b	a / b^2		
small diameter; US	89	9.7	0.946	0.240	0.254
small diameter; SFM	78	9.1	0.942	0.280	0.297
large diameter; US	50	7.5	0.889	0.072	0.081
large diameter; SFM	55	7.5	0.978	0.085	0.087

S4. References

- [SI-1] R. B. Weisman, S. M. Bachilo, Nano Lett. 3, 1235–1238 (2003). <https://doi.org/10.1021/nl034428i>
- [SI-2] I. Al-Nahhal, O. A. Dobre, E. Basar, C. Moloney, S. Ikki, IEEE Signal Process. Mag. 36, 157–163 (2019). <https://doi.org/10.1109/MSP.2019.2927685>
- [SI-3] V. Jain, M. C. Biesinger, M. R. Linford, Appl. Surf. Sci. 447, 548–553 (2018). <https://doi.org/10.1016/j.apsusc.2018.03.190>