Supporting Information to *J. Phys. Chem. C*, http://dx.doi.org/10.1021/jp4085348:

Effect of Catalyst Pretreatment on Chirality-Selective Growth of Single-Walled Carbon Nanotubes

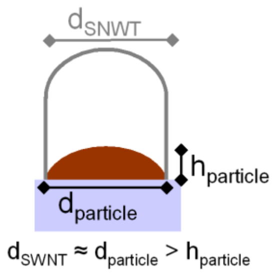
Martin Fouquet,[1,#] Bernhard C. Bayer,[1,#] Santiago Esconjauregui,[1]
Christian Thomsen,[2] Stephan Hofmann,[1] John Robertson[1]

[1]*Department of Engineering, University of Cambridge, Cambridge CB3 0FA, United Kingdom*
[2]*Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany*

[#] Equally contributed

Discussion of the particle height/nanotube diameter relationships (Figure 5 and Figure 6)

Regarding the equivalence of absolute nanotube diameter values in Figure 5 and the nanoparticle height values in Figure 6, we note that AFM-derived particle heights often only have a relative correlation (but not absolute equivalence) with measured SWNT diameters.[S1] For supported particles (as in our study) there can be a difference between the height of a particle (which is measured very accurately by AFM) and the diameter of a particle on the support (which is very inaccurately measured with AFM due to tip convolution), see sketch in Supporting Figure S1. The diameter on the support is often seen as the determining factor for nanotube diameter selection, thus particle height distributions can appear shifted to smaller values than the corresponding SWNT diameter distributions (as observed in our study). Further, Co nanoparticles inevitably oxidize during standard AFM measurements in ambient air.[S2,S3] This oxidation leads to a volume increase of the nanoparticles (Pilling-Bedworth ratio of ~2 for Co-oxide formation[S4]), further complicating the absolute relationship between measured particle heights and SWNT diameters. We also not that in our previous work in ref. S3 we had used height histograms over the total AFM-measured area to estimate particle height distributions, whereas in the present study we estimated the height distributions based on identification of individual particles in our AFM measurements. This difference in methodology accounts for the difference in estimated absolute values.



Supporting Figure S1: Schematic illustration of the relations of particle height, particle diameter and resulting nanotube diameter.

Chiral abundance analysis - raw data

Tables of all assigned (n, m) for all growth conditions. The diameter d is in nm, the RBM wave-number in cm^{-1} and the abundance in % (material fraction as measured by Raman spectroscopy).

Supporting Table 1: Table of all assigned (n, m) for C_2H_2 growth comparing vacuum and NH_3 pre-treatment. Note that the data for C_2H_2/vacuum pre-treatment is taken from ref. S3 (*Phys. Rev. B* **2012**, *85*, 235411).

C_2H_2									
vacuum-pre-treatment					NH_3-pre-treatment				
n	*m*	*d*	*abundance*	*RBM*	*n*	*m*	*d*	*abundance*	*RBM*
7	5	0.82	14.27	284.3	6	5	0.75	34.48	307.9
7	6	0.88	11.44	265.4	7	6	0.88	14.81	265.3
10	9	1.29	10.48	184.7	9	2	0.80	8.39	289.3
7	7	0.95	8.56	246.9	7	5	0.82	6.06	284.3
8	5	0.89	8.08	261.1	11	1	0.90	4.24	258.2
6	5	0.75	6.16	308.2	9	6	1.02	3.17	227.9
11	1	0.90	5.19	258.4	10	4	0.98	3.14	238.1
8	3	0.77	5.12	299.7	6	6	0.81	2.47	284.2
13	3	1.15	4.19	206.1	7	7	0.95	2.35	245.9
13	8	1.44	3.72	171.4	9	8	1.15	2.06	199.7
12	8	1.37	3.13	176.0	11	7	1.23	1.66	192.1
16	5	1.49	2.59	161.7	14	6	1.39	1.58	171.8
6	4	0.68	2.47	337.8	8	3	0.77	1.47	299.4
11	7	1.23	2.44	193.1	7	4	0.76	1.47	303.5
6	6	0.81	2.18	285.5	11	9	1.36	1.36	179.4
10	7	1.16	1.41	203.8	10	9	1.29	1.23	184.5
10	4	0.98	1.01	234.3	11	5	1.11	1.22	212.8
7	4	0.76	0.98	304.3	8	5	0.89	0.93	260.6
12	7	1.30	0.75	182.7	11	2	0.95	0.84	243.4
10	0	0.78	0.73	291.2	12	3	1.08	0.83	217.9
13	0	1.02	0.68	228.4	13	4	1.21	0.78	198.2
12	5	1.18	0.64	201.4	12	5	1.19	0.76	199.0
9	3	0.85	0.48	271.3	6	4	0.68	0.73	337.1
15	1	1.22	0.47	193.5	10	0	0.78	0.72	291.7
14	2	1.18	0.45	200.5	13	3	1.15	0.66	204.1
14	4	1.28	0.41	187.6	10	1	0.83	0.59	274.1
12	3	1.08	0.38	217.7	12	2	1.03	0.43	227.7
12	0	0.94	0.37	247.6	15	2	1.26	0.41	188.3
15	2	1.26	0.32	188.2	9	3	0.85	0.24	266.8
10	1	0.82	0.29	274.3	13	6	1.32	0.22	185.1
15	5	1.41	0.25	169.5	12	7	1.30	0.19	183.4
10	6	1.10	0.22	215.8	10	6	1.10	0.12	215.3
11	2	0.95	0.15	242.9	12	0	0.94	0.10	248.8
8	0	0.63	0.08	363.1	14	1	1.14	0.07	209.1

Supporting Table 2: Table of all assigned (n, m) for Ethanol growth comparing vacuum and NH_3 pre-treatment.

Ethanol									
vacuum-pre-treatment					NH_3-pre-treatment				
n	*m*	*d*	*abundance*	*RBM*	*n*	*m*	*d*	*abundance*	*RBM*
14	9	1.57	12.48	149.9	7	6	0.88	11.17	265.4
9	8	1.15	9.99	202.6	7	7	0.95	10.50	246.8
10	9	1.29	8.85	185.4	10	9	1.29	7.70	186.2
11	7	1.23	8.17	197.5	13	0	1.02	7.05	228.7
11	9	1.36	5.93	180.0	11	1	0.90	5.67	258.6
9	6	1.02	5.79	226.5	7	5	0.82	5.59	285.0
7	6	0.88	4.15	263.6	12	5	1.19	5.14	200.7
18	9	1.87	3.97	136.9	14	9	1.56	4.74	154.4
11	10	1.43	3.76	171.6	12	10	1.49	4.63	163.6
13	9	1.50	3.35	161.3	11	7	1.23	4.19	191.6
16	2	1.34	3.23	177.7	8	5	0.89	3.88	261.6
13	4	1.21	2.94	196.0	13	3	1.15	3.25	205.2
7	7	0.95	2.91	244.4	11	5	1.11	2.55	211.9
12	10	1.49	2.64	162.9	14	6	1.39	2.46	173.1
16	6	1.54	2.39	157.1	6	6	0.81	2.41	285.3
12	3	1.08	2.25	213.3	8	3	0.77	2.34	300.5
16	11	1.84	2.23	132.5	13	4	1.21	1.87	196.4
13	5	1.26	1.80	186.0	12	3	1.08	1.60	218.4
11	5	1.11	1.46	210.6	11	4	1.05	1.54	226.9
18	1	1.45	1.31	169.4	6	5	0.75	1.41	308.4
12	2	1.03	1.20	224.6	12	11	1.56	1.16	157.7
13	3	1.15	1.11	204.9	16	5	1.49	1.12	164.2
17	6	1.62	0.85	148.1	10	4	0.98	0.98	239.8
8	5	0.89	0.80	257.6	14	1	1.14	0.88	208.3
7	5	0.82	0.78	281.7	9	6	1.02	0.85	233.1
15	8	1.58	0.67	152.8	13	9	1.50	0.77	164.0
10	3	0.92	0.62	251.3	14	4	1.28	0.76	183.5
12	8	1.37	0.46	176.4	17	0	1.33	0.68	182.1
8	8	1.09	0.43	215.2	13	8	1.44	0.62	167.1
10	4	0.98	0.40	236.3	7	4	0.76	0.42	303.6
10	7	1.16	0.37	198.9	13	1	1.06	0.40	222.0
14	2	1.18	0.35	196.2	13	6	1.32	0.40	179.5
9	3	0.85	0.34	263.2	15	2	1.26	0.33	191.0
11	1	0.90	0.31	256.8	9	2	0.80	0.28	289.5
8	3	0.77	0.24	297.5	10	0	0.78	0.23	294.5
15	7	1.53	0.19	158.2	9	3	0.85	0.19	265.6
10	0	0.78	0.18	287.9	10	1	0.83	0.13	272.4
12	11	1.56	0.18	158.0	12	0	0.94	0.07	274.9
15	10	1.71	0.16	141.4	7	2	0.64	0.05	360.4
6	5	0.75	0.15	305.2					
13	0	1.02	0.13	228.1					
9	5	0.96	0.13	243.7					
10	8	1.22	0.12	195.1					
11	2	0.95	0.10	242.5					
12	7	1.30	0.08	182.7					
10	1	0.83	0.06	270.1					
15	2	1.26	0.02	187.8					

Supporting References

(S1) Paillet, M.; Jourdain, V.; Poncharal, P.; Sauvajol, J.-L.; Zahab, A.; Meyer, J. C.; Roth, S.; Cordente, N.; Amiens, C.; Chaudret, B. Versatile Synthesis of Individual Single-Walled Carbon Nanotubes from Nickel Nanoparticles for the Study of Their Physical Properties. *J. Phys. Chem. B* **2004**, *108*, 17112–17118.

(S2) Pisana, S.; Cantoro, M.; Parvez, A.; Hofmann, S.; Ferrari, A.; Robertson, J. The Role of Precursor Gases on the Surface Restructuring of Catalyst Films during Carbon Nanotube Growth. *Phys. E Low-Dimens. Syst. Nanostructures* **2007**, *37*, 1–5.

(S3) Fouquet, M.; Bayer, B. C.; Esconjauregui, S.; Blume, R.; Warner, J. H.; Hofmann, S.; Schlögl, R.; Thomsen, C.; Robertson, J. Highly Chiral-Selective Growth of Single-Walled Carbon Nanotubes with a Simple Monometallic Co Catalyst. *Phys. Rev. B* **2012**, *85*, 235411.

(S4) Metz, R.; Morel, J.; Delalu, H.; Ananthakumar, S.; Hassanzadeh, M. Direct Oxidation Route from Metal to Ceramic: Study on Cobalt Oxide. *Mater. Res. Bull.* **2009**, *44*, 1984–1989.