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APPENDICES

Appendix A

Finding the volume of manifold and cylinder

Calculation procedure

In order to calibrate dead volume of the apparatus, the mass balance was taken between the two states. The first state was the initial state, before expansion. The second state was after expansion into the cylinder. After that, two mass balance equations for with and without known volume were solved and the volume of manifold and sample cylinder will be obtained.

Known volume (stainless steel)

Density of steel (g/cc) is 7.7728 g/cc

Weight of steel in this experiment is 38.9528 g

Known volume is 5.01 cc

Table A1 Pressure data for calculate volume space of the apparatus.

Run	Condition	Pressure (psia)			
		Blank		Steel contained	
		initial	final	initial	final
1	He at 126 psia	126.1432	93.7430	126.9407	97.3340
2	He at 226 psia	226.2792	169.9451	226.4862	174.4970
3	He at 326 psia	326.0366	248.5621	326.8404	254.9990
4	He at 426 psia	426.1905	321.5217	425.3753	329.0219
5	He at 526 psia	526.1609	397.5140	525.1270	406.4430
6	He at 626 psia	626.3680	473.6502	624.0815	483.2760
7	He at 726 psia	726.3088	548.9280	725.5465	561.4841
8	He at 826 psia	825.7532	623.5637	826.3384	639.3681
9	He at 926 psia	925.8418	699.0810	926.0900	715.9011
10	He at 1026 psia	1026.1136	778.3883	1026.5215	793.9349
11	He at 1126 psia	1126.1787	849.5349	1126.0427	870.1256

Table A2 Density of Helium gas to calculate volume space of the apparatus.

Run	Condition	Density (g/cc)			
		Blank		Steel contained	
		initial	final	initial	final
1	He at 126 psia	0.0007	0.0005	0.0007	0.0005
2	He at 226 psia	0.0013	0.0009	0.0013	0.0010
3	He at 326 psia	0.0018	0.0014	0.0018	0.0014
4	He at 426 psia	0.0024	0.0018	0.0024	0.0018
5	He at 526 psia	0.0029	0.0022	0.0029	0.0022
6	He at 626 psia	0.0034	0.0026	0.0034	0.0027
7	He at 726 psia	0.0040	0.0030	0.0040	0.0031
8	He at 826 psia	0.0045	0.0034	0.0045	0.0035
9	He at 926 psia	0.0050	0.0038	0.0050	0.0039
10	He at 1026 psia	0.0056	0.0042	0.0056	0.0043
11	He at 1126 psia	0.0061	0.0046	0.0061	0.0047

Table A3 Volume of manifold and sample cylinder.

Pressure	Vm	Vs
126	121.425077	41.77661
226	150.594239	49.51472
326	169.193215	52.12457
426	155.666505	49.91388
526	161.511007	51.30665
626	165.006607	52.04477
726	166.15247	52.34586
826	162.068096	51.06508
926	168.166517	52.83243
1026	205.179059	63.03976
1126	165.2224	51.77487

	Vm	Vs
average	162.4304143	51.88787508

Appendix B

Calculation for the adsorbed hydrogen

The gas density at any pressure and temperature was calculated by Beattie-Bridgeman Equation of State.

$$P = \frac{R_u T}{\upsilon^2}\left(1 - \frac{c}{\upsilon T^3}\right)(\upsilon + B) - \frac{A}{\upsilon^2}$$

$$A = A_0\left(1 - \frac{a}{\upsilon}\right), \quad B = B_0\left(1 - \frac{b}{\upsilon}\right)$$

Table B1 Parameter for Beattie-Bridgeman Equation.

	Hydrogen	psia	Kpa				
	Preal		6652.3584				
	Ru		8.314	Kpa*m^3/kmolK			
	T		298	K			
	T^3		26463592	K			
time	A	B	Ao	a	Bo	b	c
initial	20.273362	0.0233209	20.0117	-0.00506	0.02096	-0.04359	504
0:00:00	20.26215855	0.0232198					
0:05:10	20.2619986	0.0232184					
0:10:20	20.26184858	0.0232171					
0:30:30	20.26149751	0.0232139					
1:00:40	20.2608633	0.0232082					
1:30:50	20.26017254	0.0232019					
2:01:00	20.25942187	0.0231952					
3:01:10	20.25832653	0.0231853					
6:01:20	20.25547865	0.0231596					
9:01:30	20.25123926	0.0231213					
12:01:40	20.24710324	0.023084					
15:01:50	20.24292742	0.0230463					
18:02:00	20.23897195	0.0230106					
21:02:10	20.23503038	0.0229751					

	H2 gas	He gas
A0	20.0117	2.1886
B0	0.02096	0.05984
a	-0.00506	0.014
b	-0.04359	0
c	504	40

The calculation is done on Excel program. Then, the amount of hydrogen remained in sample cylinder was calculated.

Table B2 Calculated density from Beattie-Bridgeman Equation

time	P experiment	P(v) cal	V(p) cal	Density cal
initial	964.8430492	964.843	0.38698	0.00521
0:00:00	921.833	921.833	0.4043	0.004986
0:05:10	921.2201724	921.22	0.40455	0.004983
0:10:20	920.6454516	920.645	0.4048	0.00498
0:30:30	919.300595	919.301	0.40537	0.004973
1:00:40	916.8715304	916.871	0.4064	0.004961
1:30:50	914.2265138	914.226	0.40753	0.004947
2:01:00	911.3528287	911.353	0.40876	0.004932
3:01:10	907.1610139	907.161	0.41058	0.00491
6:01:20	896.2699389	896.27	0.41537	0.004853
9:01:30	880.077518	880.077	0.42272	0.004769
12:01:40	864.3030644	864.303	0.43015	0.004687
15:01:50	848.3998525	848.4	0.43792	0.004604
18:02:00	833.3570796	833.357	0.44554	0.004525
21:02:10	818.3875828	818.388	0.45341	0.004446

Correction methods for hydrogen adsorption

Subtraction method

Step 1. The calculated hydrogen amount was employed by using the Equation of state in both experiments blank test and adsorbed test.

Pressure (blank test) density amount of hydrogen leaking A

Pressure (adsorbed test) density amount of adsorption B

Step 2. The correction of hydrogen amount was achieved by adding an amount of hydrogen leakage (from blank test) to adsorbed test data. Therefore, the adsorbed data was already done away with the effect of leaking.

Amount of adsorption C = A+B

Step 3. The amount of hydrogen adsorption was calculated by the new adsorbed data. The adsorbed amount was performed in term of hydrogen percentage.

Amount of adsorption C % hydrogen

Pressure correction factor

Step 1. The pressure correction factor was the factor of pressure at that time per initial pressure, which obtained from blank test.

Pressure at that time / initial pressure = pressure correction factor

Step 2. The correction of pressure was achieved by multiplying the pressure correction factor with the pressure obtained from pressure transducer.

Step 3. The amount of hydrogen adsorption was reported in percent hydrogen adsorbed on the adsorbent (wt basis).

Appendix C

Metal contents in the carbon nanotubes samples

Table C1 Trace metals analysis results (wt%).

	MWNT(31522-8)	SWNT(31522-9)
As	<0.01	<0.01
Ca	0.0039	0.027
Co	0.88	24.3
Cr	0.0012	<0.001
Cu	<0.001	<0.001
Fe	0.478	<0.001
Pb	<0.002	0.017
Mg	<0.001	0.058
Mn	<0.001	0.001
Mo	<0.001	<0.001
Na	0.025	0.026
Ni	0.0086	0.037
Pb	0.002	<0.002
Si	<0.002	N/A
Sn	<0.01	<0.01
Ti	<0.001	0.003
V	<0.001	0.001
Zn	<0.001	<0.001
Al	2.83	0.02
B	<0.001	<0.001
Cd	<0.001	<0.001
Ga	<0.002	<0.002
K	<0.002	0.008
Li	<0.0002	<0.0002
Nb	<0.002	0.002
Pd	<0.001	<0.001
Pt	<0.001	<0.001
Rh	<0.001	<0.001
Sb	<0.001	<0.001
Sr	<0.001	<0.001
Ta	<0.002	<0.002
Zr	<0.001	<0.001

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