Supplementary information for

ReaxFF MD simulations of graphitization of intact and O,N-doped amorphous carbon

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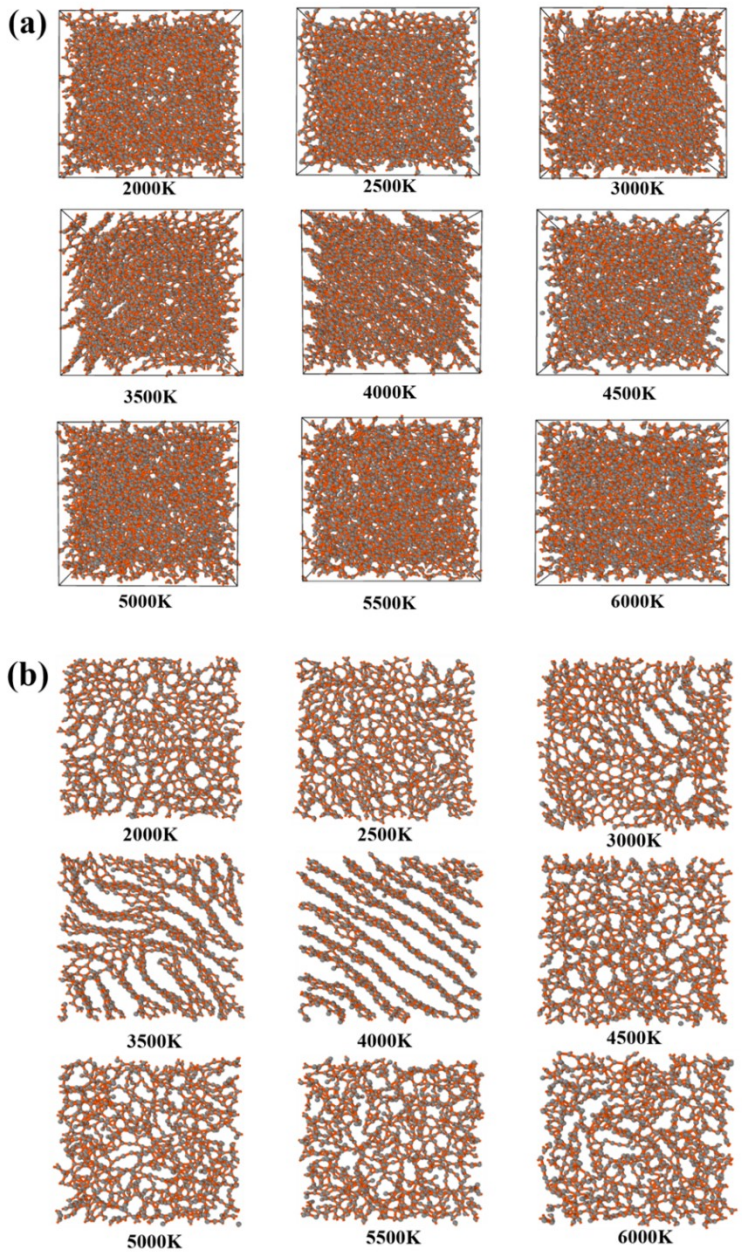

Figure S1. Graphitized structures obtained at different annealing temperatures: (a) the full systems (32 Å in thickness); (b) sliced views with a thickness of 10 Å.

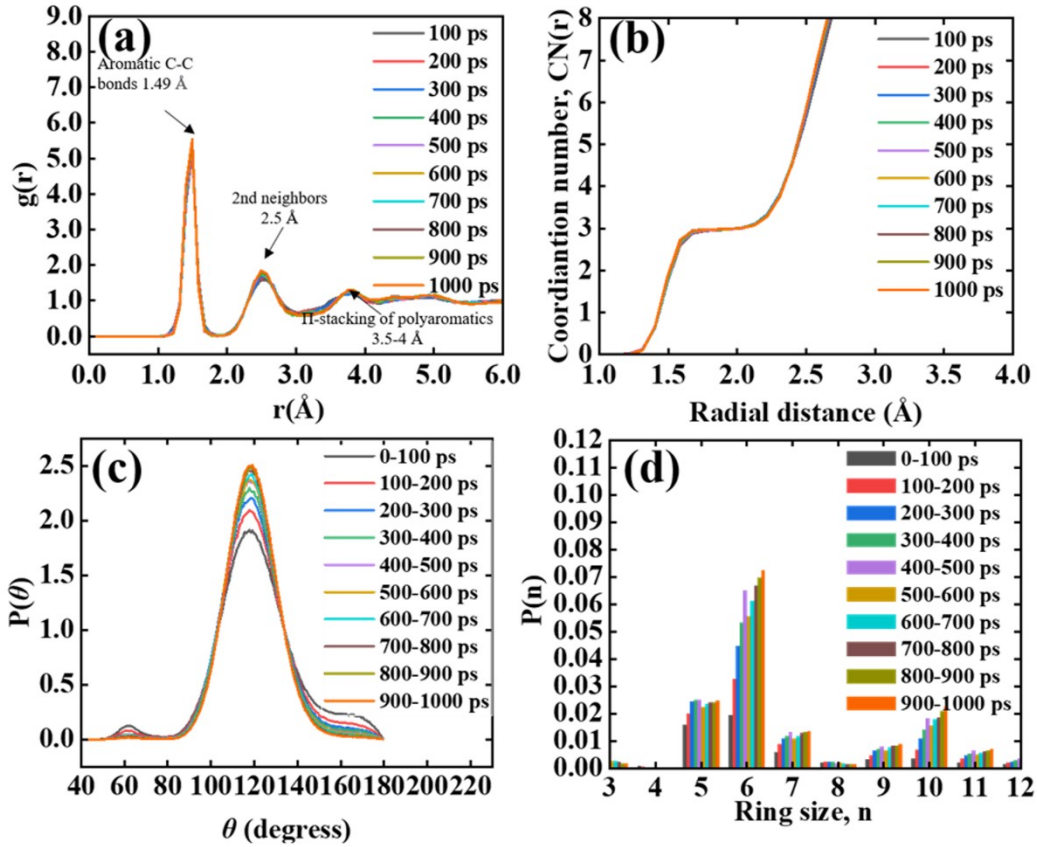

Figure S2. Structural characterization of amorphous carbon at the different stages of simulation at the annealing temperature of 3500 K. (a) C-C RDFs; (b) coordination number of C atoms; c) C-C-C bond angle distribution; (d) ring distribution

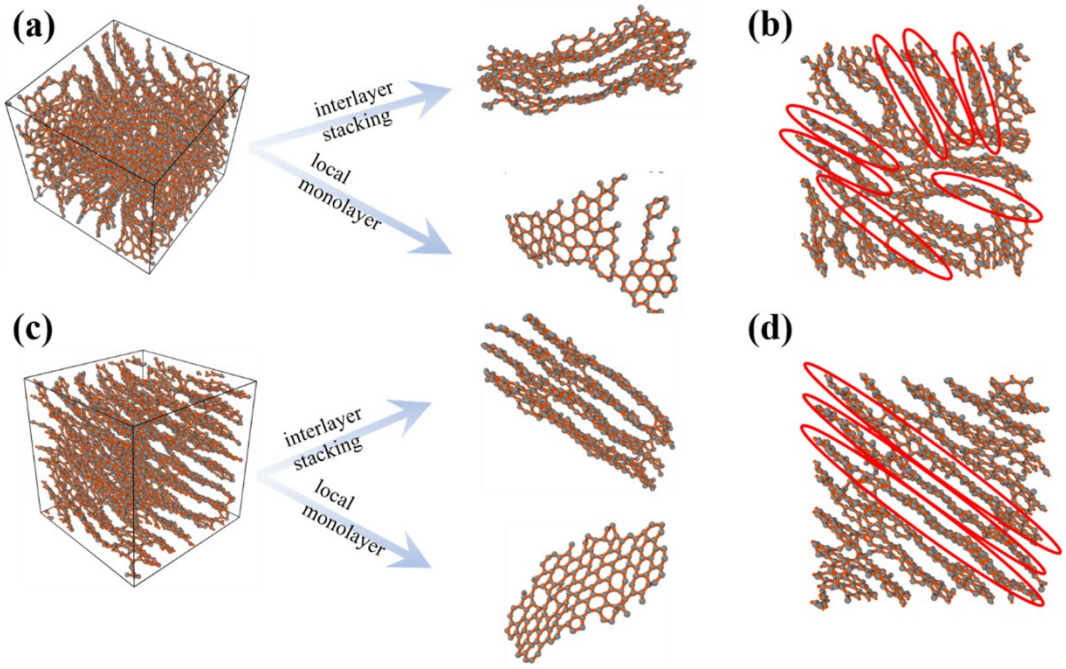

Figure S3. Local structure (a) and slice (b) of amorphous carbon annealed at 3500 K; local structure (c) and slice (d) of amorphous carbon annealed at 4000 K. Comparing

the graphitized structures of amorphous carbon annealed at 3500 K and 4000 K, it is observed that the graphite-like layered structure after annealing at 4000 K is more orderly arranged with consistent orientation. The number of six-membered rings in the monolayer structure is significantly higher than that at 3500 K. Additionally, in both cases, the layers are connected through interactions between in-plane atoms and carbon atoms of adjacent layers.

ReaxFF used in this work:

39 ! Number of general parameters
50.0000 !Overcoordination parameter
9.4514 !Overcoordination parameter
30.0000 !Valency angle conjugation parameter
216.4305 !Triple bond stabilisation parameter
12.4838 !Triple bond stabilisation parameter
0.0000 !C2-correction
1.0701 !Undercoordination parameter
7.5000 !Triple bond stabilisation parameter
11.9083 !Undercoordination parameter
13.3822 !Undercoordination parameter
-10.4637 !Triple bond stabilization energy
0.0000 !Lower Taper-radius
10.0000 !Upper Taper-radius
2.8793 !Not used
33.8667 !Valency undercoordination
3.5895 !Valency angle/lone pair parameter

1.0563 !Valency angle
2.0384 !Valency angle parameter
6.1431 !Not used
6.9290 !Double bond/angle parameter
0.0283 !Double bond/angle parameter: overcoord
0.0570 !Double bond/angle parameter: overcoord
-2.4837 !Not used
5.8374 !Torsion/BO parameter
10.0000 !Torsion overcoordination
1.8820 !Torsion overcoordination
-1.2327 !Conjugation 0 (not used)
2.1861 !Conjugation
1.5591 !vdWaals shielding
0.0100 !Cutoff for bond order (*100)
5.2216 !Valency angle conjugation parameter
3.4021 !Overcoordination parameter
38.5241 !Overcoordination parameter
2.1533 !Valency/lone pair parameter
0.5000 !Not used
20.0000 !Not used
5.0000 !Molecular energy (not used)
2.0000 !Version number
6.5560 !Valency angle conjugation parameter
4 ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.
ov/un;val1;n.u.;val3,vval4
C 1.3742 4.0000 12.0000 1.9684 0.1723 0.8712 1.2385 4.0000
9.4606 2.1346 4.0000 31.0823 79.5548 5.7254 6.9235 0.0000
1.2104 0.0000 183.7012 5.7419 33.3951 11.9957 0.8563 0.0000
-2.8983 2.5000 1.0564 4.0000 2.9663 0.0000 0.0000 0.0000
H 0.6867 1.0000 1.0080 1.3525 0.0616 0.8910 -0.1000 1.0000
9.3858 5.0013 1.0000 0.0000 121.1250 3.8446 10.0839 1.0000
-0.1000 0.0000 58.4228 3.8461 3.2540 1.0000 1.0698 0.0000
-15.7683 2.1504 1.0338 1.0000 2.8793 0.0000 0.0000 0.0000
O 1.3142 2.0000 15.9990 1.9741 0.0880 0.8712 1.1139 6.0000
10.2186 7.7719 4.0000 29.5271 116.0768 8.5000 7.1412 2.0000
0.9909 14.9473 69.2812 9.1371 1.6258 0.1863 0.9745 0.0000
-3.5965 2.5000 1.0493 4.0000 2.9225 0.0000 0.0000 0.0000
N 1.2450 3.0000 14.0000 1.9951 0.1088 1.0512 1.1911 5.0000
9.9303 7.8431 4.0000 32.4758 100.0000 6.7768 6.8035 2.0000
1.0636 0.1045 128.0119 2.1604 2.9464 2.5181 0.9745 0.0000
-4.0959 2.0047 1.0183 4.0000 2.8793 0.0000 0.0000 0.0000
10 ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6

pbe2;pbo3;pbo4;Etrip;pbo1;pbo2;ovcorr
1 1 141.9346 113.4487 67.6027 0.1554 -0.3045 1.0000 30.4515 0.4283
0.0801 -0.2113 8.5395 1.0000 -0.0933 6.6967 1.0000 0.0000
1 2 163.6889 0.0000 0.0000 -0.4525 0.0000 1.0000 6.0000 0.5921
12.1053 1.0000 0.0000 1.0000 -0.0097 8.6351 0.0000 0.0000
2 2 169.8421 0.0000 0.0000 -0.3591 0.0000 1.0000 6.0000 0.7503
9.3119 1.0000 0.0000 1.0000 -0.0169 5.9406 0.0000 0.0000
1 3 164.0476 117.4881 72.1261 -0.6031 -0.1795 1.0000 14.9755 0.5413
1.2626 -0.3063 7.0000 1.0000 -0.1588 4.5000 0.0000 0.0000
3 3 110.4748 155.6441 40.0000 0.1150 -0.1054 1.0000 28.5221 0.2000
0.9590 -0.2635 8.5715 1.0000 -0.1007 6.8548 1.0000 0.0000
1 4 130.7147 175.2276 97.2523 -0.0368 -0.4942 1.0000 26.7545 0.5133
0.3296 -0.3653 7.0000 1.0000 -0.1171 5.1025 1.0000 0.0000
3 4 85.4950 114.0081 70.1453 0.5778 -0.1070 1.0000 16.6611 0.2339
0.3474 -0.1948 8.3762 1.0000 -0.1089 5.8148 1.0000 0.0000
4 4 157.7518 67.1322 160.9732 -0.5869 -0.1824 1.0000 12.0000 0.7136
0.8204 -0.1657 10.6490 1.0000 -0.0967 4.5976 1.0000 0.0000
2 3 224.3076 0.0000 0.0000 -0.6280 0.0000 1.0000 6.0000 1.0000
5.0050 1.0000 0.0000 1.0000 -0.0512 5.1982 0.0000 0.0000
2 4 212.1772 0.0000 0.0000 -0.3585 0.0000 1.0000 6.0000 0.3316
10.4316 1.0000 0.0000 1.0000 -0.0658 6.4545 0.0000 0.0000
6 ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
1 2 0.0464 1.8296 10.1311 1.0029 -1.0000 -1.0000
2 3 0.0375 1.7275 10.8037 0.8813 -1.0000 -1.0000
2 4 0.0509 1.7672 10.4261 0.9990 -1.0000 -1.0000
1 3 0.1036 1.8869 9.5668 1.3590 1.1099 1.1534
1 4 0.1971 1.7356 10.0734 1.2754 1.2113 1.1172
3 4 0.0535 1.6709 10.8180 1.2968 1.1416 1.0167
42 ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
1 1 1 74.0317 32.2712 0.9501 0.0000 0.1780 10.5736 1.0400
1 1 2 70.6558 14.3658 5.3224 0.0000 0.0058 0.0000 1.0400
2 1 2 76.7339 14.4217 3.3631 0.0000 0.0127 0.0000 1.0400
1 2 2 0.0000 0.0000 6.0000 0.0000 0.0000 0.0000 1.0400
1 2 1 0.0000 3.4110 7.7350 0.0000 0.0000 0.0000 1.0400
2 2 2 0.0000 27.9213 5.8635 0.0000 0.0000 0.0000 1.0400
1 1 3 65.3104 6.3897 7.5000 0.0000 0.2000 10.0000 1.8525
3 1 3 71.9855 28.5708 6.4252 0.0000 0.2000 0.0000 1.8525
1 1 4 65.8892 45.0000 1.6598 0.0000 0.2000 10.0000 1.8525
3 1 4 73.1057 25.8227 4.2145 0.0000 0.2000 0.0000 1.8525
4 1 4 65.8759 40.9838 2.4369 0.0000 0.2000 0.0000 1.8525
2 1 3 56.3039 17.3681 5.3095 0.0000 0.9110 0.0000 1.0400
2 1 4 71.5505 11.1820 3.7129 0.0000 0.9110 0.0000 1.0400
1 2 4 0.0000 0.0019 6.3000 0.0000 0.0000 0.0000 1.0400
1 3 1 72.3642 37.8942 1.1566 0.0000 0.7472 0.0000 1.2639

1 3 3 90.0000 45.0000 0.5719 0.0000 0.7472 0.0000 1.2639
1 3 4 70.4313 14.4055 7.1593 0.0000 0.7472 0.0000 1.2639
3 3 3 83.8833 23.3345 2.3433 -10.0000 0.7472 0.0000 1.2639
3 3 4 84.0407 45.0000 1.0695 0.0000 0.7472 0.0000 1.2639
4 3 4 73.9966 24.4410 5.2760 0.0000 0.7472 0.0000 1.2639
1 3 2 89.1394 37.0874 0.3849 0.0000 3.0000 0.0000 1.2618
2 3 3 80.7068 5.0854 5.7151 0.0000 3.0000 0.0000 1.2618
2 3 4 76.0238 45.0000 0.8637 0.0000 3.0000 0.0000 1.2618
2 3 2 82.3474 13.5165 3.4896 0.0000 0.3596 0.0000 1.3307
1 4 1 68.4330 19.3525 2.1625 0.0000 1.7325 0.0000 1.0440
1 4 3 86.2893 37.5587 1.2660 0.0000 1.7325 0.0000 1.0440
1 4 4 74.2404 12.0547 7.5000 0.0000 1.7325 0.0000 1.0440
3 4 3 78.5566 43.8492 1.3351 -26.1471 1.7325 40.0000 1.0440
3 4 4 77.4239 33.7297 1.7944 -0.9193 1.7325 0.0000 1.0440
4 4 4 64.9107 17.5558 7.5000 0.0000 1.7325 0.0000 1.0440
1 4 2 90.0000 32.0540 0.7195 0.0000 0.5355 0.0000 2.5279
2 4 3 84.1185 45.0000 1.3826 0.0000 0.5355 0.0000 2.5279
2 4 4 78.7133 24.6250 3.8202 0.0000 0.5355 0.0000 2.5279
2 4 2 56.3036 14.1532 3.3914 0.0000 0.2000 0.0000 2.1689
1 2 3 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
1 2 4 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
1 2 5 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
3 2 3 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
3 2 4 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
4 2 4 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
2 2 3 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
2 2 4 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
17 ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
1 1 1 1 0.0000 48.4194 0.3163 -8.6506 -1.7255 0.0000 0.0000
1 1 1 2 0.0000 63.3484 0.2210 -8.8401 -1.8081 0.0000 0.0000
2 1 1 2 0.0000 45.2741 0.4171 -6.9800 -1.2359 0.0000 0.0000
0 1 2 0 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
0 2 2 0 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
0 1 3 0 -0.0002 85.8794 0.3236 -3.8134 -2.0000 0.0000 0.0000
0 2 3 0 0.0000 0.1000 0.0200 -2.5415 0.0000 0.0000 0.0000
0 3 3 0 -0.9667 116.4743 0.0002 -4.9422 0.0000 0.0000 0.0000
0 1 4 0 -0.0069 150.0000 0.4891 -7.4921 -2.0000 0.0000 0.0000
0 2 4 0 0.0000 0.1000 0.0200 -2.5415 0.0000 0.0000 0.0000
0 3 4 0 1.6745 56.6301 -0.0008 -4.5064 -2.0000 0.0000 0.0000
0 4 4 0 1.1253 75.3447 0.0080 -9.0000 -2.0000 0.0000 0.0000
0 1 1 0 0.0930 18.5962 0.0002 -9.0000 -1.0000 0.0000 0.0000
4 1 4 4 -2.0000 20.8732 -1.5000 -9.0000 -2.0000 0.0000 0.0000
1 1 3 3 -0.0002 21.5452 0.1727 -9.0000 -2.0000 0.0000 0.0000
1 3 3 1 0.0002 79.3777 -1.5000 -5.2139 -2.0000 0.0000 0.0000

```
3   1   3   3   -1.3476   22.4932    1.5000   -9.0000   -2.0000    0.0000    0.0000
4       ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
3   2   3    2.0000   -5.0000    3.0000    3.0000
3   2   4    1.7753   -5.0000    3.0000    3.0000
4   2   3    1.3884   -5.0000    3.0000    3.0000
4   2   4    1.6953   -4.0695    3.0000    3.0000
```