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Supplementary Information

Effect of N doping on the microstructure and dry etch properties of amorphous

carbon deposited with a DC sputtering system

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Fig. S1.(a) A schematic of the DC sputtering system. (b) deposition rate of amorphous carbon film according to nitrogen concentration.

Fig. S2.XPS plot of amorphous carbon according to its plasma gas ratio (a) wide scan, (b) C1s scan (c) N1s scan.

Area $%$	C1s					O1s			
	C-C $\begin{array}{ c c c c c } \hline \text{C-C}_{\text{high}} & \text{C-O} \ \hline & & & \text{C}_{\text{sp2-N}} \ \hline & & & \text{C}_{\text{sp2-N}} \ \hline \end{array}$			$C = O$	$C(O)-O$	$O-N$	$O-C$	$O-C$	$O=C$
								aliphatic	
N 3.2 at%	26.7	46.5	14.5	6.8	5.5	6.6	42.6	23.6	25.6
N 9.0 at%	25.4	45.8	14.6	9	5.2	31.2	21.2	21.6	22.4
N 11.1 at%	25.6	47.2	14.1	7.5	5.6	36.7	18.0	18.6	20.9

Table S1. Percentage of peak composition of C1s and O1s peaks acquired from Fig S2(b) and $S2(c)$.

Fig. S3. XRR plot of amorphous carbon according to its plasma gas ratio.

Fig. S4. RDF(Radial distribution function) plot of amorphous carbon according to its plasma gas ratio.

Fig. S5. FIB cross section image of the amorphous carbon films (a, b) N 3.2 at% (a) as deposited, (b) etched, (c, d) N 9.0 at% (c) as deposited, (d) etched, (e, f) N 11.1 at% (e) as deposited, (f) etched.

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Supplementary Discussion

The difference in the position of the nitrogen in the nitrogen-doped amorphous carbon film, i.e., the chemical bonding of nitrogen can be identified not only N1s spectrum but also C1s and O1s spectrum in XPS. However, as one can see in Supplementary Fig. S2(b), it is hard to distinguish the difference in the C1s spectra and deconvolution results of each film. Compared to the Cls spectrum result, O1s spectrum (Supplementary Fig. $S_2(c)$) seems to have differences between the films. However, it should be noted that the intensity of the O1s spectrum is much lower (Supplementary Fig. S2(a)) compared to that of the Cls and N1s spectrum, as can be inferred from the noise-like form. Supplementary Table S1 describes the area fraction of the deconvolved Cls and O1s spectra of each film. One can see that the values in the C1s columns are merely varied. Also, the binding energy values of C_{sp2} -N (284.8-285.5 eV) and C_{sp3} -N(285.9-286.5 eV), which are the clues of the position of the nitrogen in the amorphous carbon films, are quite similar to that of C- $C_{\text{high}}(284.8-285.5 \text{ eV})$ and $C-O(285.9-286.5 \text{ eV})$, respectively. [1] Therefore, it is hard to extract the exact area fraction of the C-N bondings. The area fraction of the deconvolved O1s spectrum of each film varies with the amorphous carbon films, especially the amount of N-O increases as the amount of N in the amorphous carbon film increases. However, since the amount of oxygen in the film is very small, it may be expected that the effect of Sungtae Kim

the N-O bond on the properties of the carbon film would be insignificant compared to the N-C bond. As such, it is difficult to distinguish the difference in nitrogen positions in the C1s results, and the O1s results are very small, so we analyzed the N1s spectrum in depth to determine the position of nitrogen in the carbon film. In addition, we directly analyzed the bond length to clarify the position of nitrogen in the carbon film by obtaining the distance of the nearest neighbor through RDF analysis.

References

[1] M. Ayiania, M. Smith, A. J. R. Hensley, L. Scudiero, J. S. McEwen and M. Garcia-Perez, Deconvoluting the XPS spectra for nitrogen-doped chars: An analysis from first principles, Carbon, 2020, 162, 528–544.