Electrochemical Intercalation of Li into Graphite-like Layered Material BC_6N

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1. Introduction

Among many candidates for anode material of Li ion battery [1], graphite or non-crystalline carbon has been practically used. Although graphite intercalation compound of Li (Li-GIC) has advantages of low potentials, relatively high capacity (372mAh/g), *etc*., it has several disadvantages such as volume expansion after charge/discharge cycle, limited usage of solvent (propylene carbonate: PC can not be used), *etc*. We reported that Li could be intercalated into the boron/carbon/nitrogen (B/C/N) material with graphite-like layered structure in the PC [2].

In the present study, we have investigated the electrochemical intercalation of Li into the layered material with a composition of BC_6N. The volume expansion of fully intercalated material was evaluated by X-ray diffraction method.

2. Experimental

The material BC_6N was deposited on a carbon suscepter by the reaction of acrylonitrile and boron trichloride (mole ratio 2:1) at a temperature between 1470K and 2070K under atmospheric pressure [3].

Electrochemical intercalation of lithium ion into BC_6N and graphite was performed in 1.0M-$LiPF_6$ with a mixed solvent of ethylene carbonate and diethyl carbonate (EC : DEC = 1 : 1) by using two electrode cell (CE, RE: Li). X-ray diffraction (XRD) was performed for the intercalated material by using polyethylene wrapping film.

3. Results and discussion

Figure 1 shows the galvanostatic charge/discharge curves for the BC_6N prepared at 1470K. Lower potentials were observed for the discharge curves in a similar manner to that of graphite. The first charge and discharge capacities were 400mAh/g and 305mAh/g, respectively (coulombic efficiency: 77%). The second ones were 355 and 330mAh/g (90%).

Figure 2 shows XRD patterns of Li intercalated BC_6N, Li-GIC, and original host materials. Table 1 indicates the interlayer spacings (d-spacings) of the materials and the increase in d-spacing after the Li intercalation. The BC_6N obtained at 1470K and 2070K had the d-spacings of 0.339 and 0.343nm, respectively. The lower preparation temperature made the d-spacing of BC_6N smaller with higher crystallinity in this temperature range. Li intercalated BC_6N had smaller d-spacings than that of Li-GIC, as is indicated in Table 1. The degree of expansion after the Li intercalation was smaller for the Li intercalated BC_6N than that for Li-GIC. Particularly the BC_6N prepared at lower temperature (1470K) showed that the degree of expansion was half of that for graphite. Interaction between the host BC_6N and the guest Li should be important and will be further investigated. This small volume expansion is one of the advantages of BC_6N as the anode material of Li ion battery.

References

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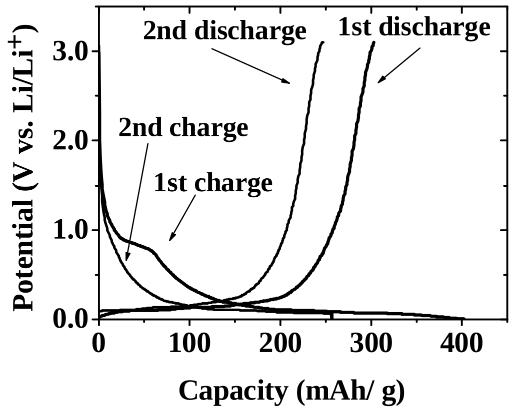

Figure 1 Charge/discharge curves of BC_6N prepared at 1470K in 1M $LiPF_6$/ (EC+DEC) electrolyte by using two electrode cell.

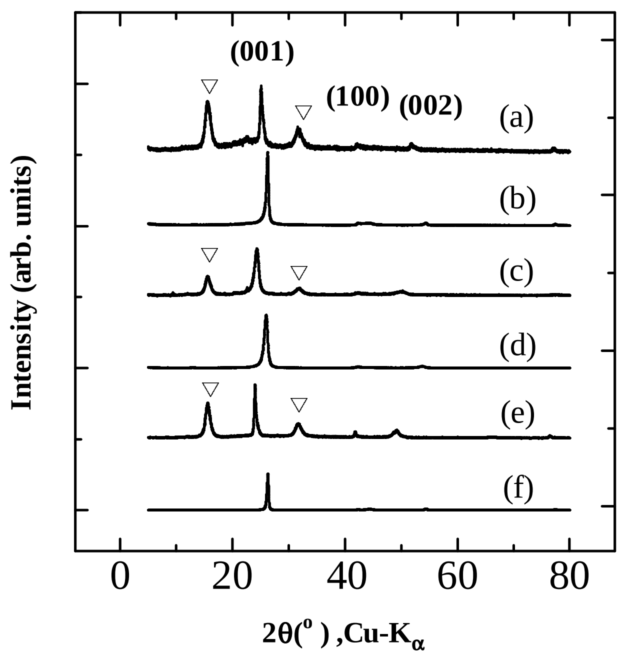

Figure 2 XRD patterns of (a) Li intercalated BC_6N [1470K], (b) the original BC_6N prepared at 1470K, (c) Li intercalated BC_6N [2070K], (d) the original BC_6N prepared at 2070K, (e) Li-GIC, and (f) graphite.
Δ: wrapping film.

Table 1 The interlayer spacings (d-spacings) of the materials and the increase in d-spacing after the Li intercalation.

Sample	(a) Original d-spacing (nm)	(b) d-spacing after intercalation (nm)	The increase in d-spacing (%) 100(b - a) /a
BC_6N prepared at 1470K	0.339	0.355	4.7
BC_6N prepared at 2070K	0.343	0.365	6.4
Graphite	0.338	0.370	9.5