Application Note B-XRD1150

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B-XRD1150 - Evaluation of graphitization degree of lithium-ion battery carbon anode material by X-ray diffractometry

Introduction

Lithium-ion batteries are becoming essential in our daily lives because they are used everywhere, such as in mobile phones, smartphones, electric vehicles, and so on. A lithium-ion battery mainly consists of a cathode, an anode, a separator and an electrolyte. The anode, in particular, seriously affects the discharge capacity, energy density and safety of the battery. Carbon is widely used as an anode material, and it influences the discharge capacity of the battery depending on the degree of the development of the graphite structure (graphitization degree). In this example, we evaluated the graphitization degree of carbon anode materials by analyzing the lattice constants and crystallite sizes, conforming to JIS R7651:2007. X-ray diffraction patterns were obtained using a compact X-ray diffractometer equipped with a high-resolution and high-speed one-dimensional detector.

Measurement and results

To evaluate the degree of graphitization, we used three carbon samples (A, B and C) prepared under different firing conditions. 10 mass% Si was added as an internal standard to these carbon samples to correct angles and widths of the diffraction peaks. Figure 1 shows the X-ray diffraction patterns of the carbon samples. No crystalline carbon peaks were observed in the XRD pattern of sample A, but they were observed in samples B and C.

Lattice spacings d_{002}, lattice constants c_0 and crystallite sizes L_{002} are shown in Table 1. The lattice spacings d_{002} and the lattice constants c_0 were calculated using integrated X-ray analysis software SmartLab Studio II; the lattice constants c_0 were determined by doubling the lattice spacing d_{002}. It is known that highly graphitized carbon tends to have a smaller lattice spacing (narrower carbon layer) and larger crystallite size (higher crystallinity). Considering this, since the lattice spacings d_{002} are larger in the order C < B < A and the crystallite sizes L_{002} are A < B < C as shown in Table 1, it is suggested that the graphitization degree is larger in the order A < B < C. Table 1 also shows the results of graphitization degrees (P_1) calculated using the following equation [(1),(2)]: $d_{002} = 3.354P_1 + 3.44(1 - P_1)$. In summary, an X-ray diffractometer allows you to evaluate the graphitization degree of carbon anode materials by analyzing the lattice constants and crystallite sizes.

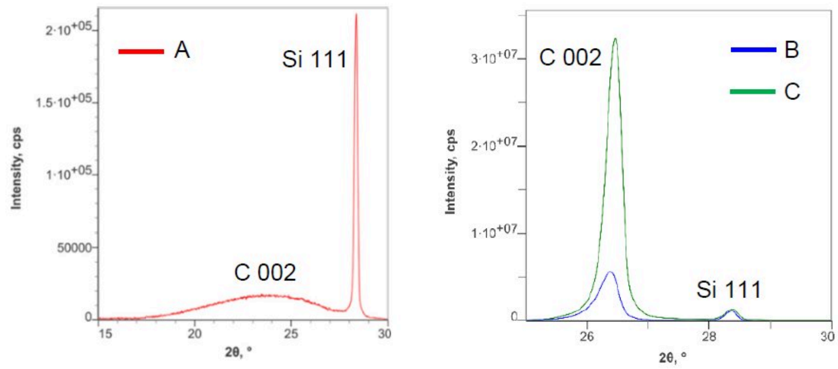

Figure 1: X-ray diffraction patterns of carbon samples A, B and C

Table 1: Graphitization degree of the carbon samples A, B and C

Carbon samples	d_{002} (Å)	c_0 (Å)	L_{002} (Å)	P_1
A	3.44	6.88	14	0
B	3.371	6.742	575	0.76
C	3.363	6.726	1587	0.85

d_{002}: average lattice spacing
c_0: lattice constant
L_{002}: crystallite size
P_1: graphitization degree

References

(1) M. Inagaki, M. Shiraishi, M. Nakamizo and Y. Hishiyama: *Tanso*, **118**(1984), 165-175 (In Japanese).
(2) T. Noda, M. Iwatsuki, M. Inagaki: *Tanso*, **47**(1966), 14-23 (in Japanese).

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