Surface Stability of Mg_3Bi_2 Zintl Phase as Negative Electrode for Magnesium-ion Batteries

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Rechargeable magnesium batteries are expected as potential beyond lithium ion systems, because of their high theoretical capacity densities owing to the divalent magnesium ion. One of the biggest challenges of the magnesium-based negative electrode is passivation of the electrode surface. The surface of the magnesium metal negative electrodes can be easily passivated in conventional electrolyte solutions, containing magnesium salts and organic solvents. We have been working on a magnesium-based intermetallics Mg_3Bi_2 Zintl phase as anodes for the magnesium-ion batteries, because the Mg_3Bi_2 anode is highly reversible in conventional ionic electrolyte solutions such as magnesium bis(trifluoromethane sulfonyl amide) ($Mg(TFSA)_2$) in acetonitrile (AN) as shown in Fig. 1 [1].

Here we evaluated the stability of the passivation layer of Mg_3Bi_2 anode and compared with Mg_3Sb_2, whose crystal structure is mostly same as that of Mg_3Sb_2. Fig. 2 shows XRD patterns of the Mg_3Bi_2 powder in ambient atmosphere and wet condition. The hydrolysis of Mg_3Bi_2, to form $Mg(OH)_2$ and Bi. It shows that the Mg_3Bi_2 does not form a stable SEI layer. On the other hand, the Mg_3Sb_2 is very stable even in a water. The results suggest that the instability of the Mg_3Bi_2 could be a key materials property for the electrochemical reversibility of the intermetallic anodes.

Further DFT modeling of the Mg_3Bi_2 was also carried out to analyze the ionic conductive properties of Mg^{2+} ions in the intermetallic phase.

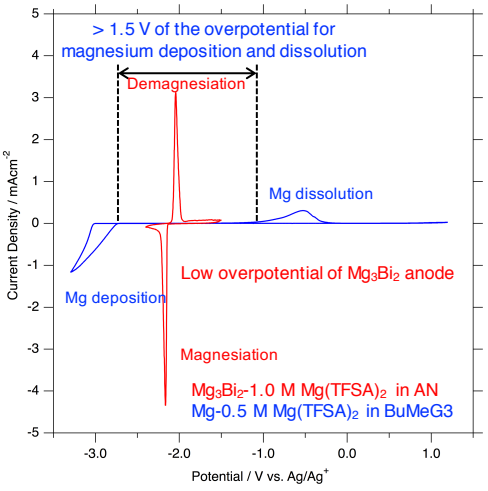

Fig. 1 Electrochemimcal property of Mg_3Bi_2 anodes.

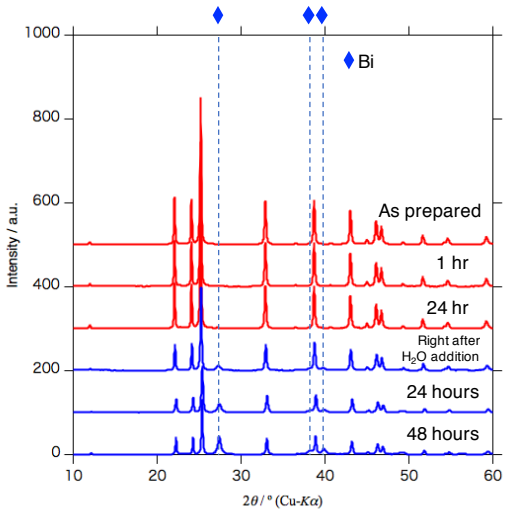

Fig. 2 XRD patterns of Mg3Bi2 powders in air

References:

[1] T. S, Arthur, N. Singh and M. Matsui, *Electrochemistry Communications*, **16**, 103 (2012).