

Electronic Supplementary Information

Anode Properties of Magnesium Hydride Catalyzed with Niobium Oxide for All Solid-State Lithium-Ion Battery

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Experimental

The solid electrolyte 80Li₂S-20P₂S₅ was synthesized through following procedure. The mixture of Li₂S (Furuuchi Chemistry, 99.9%) and P₂S₅ (Sigma Aldrich, 99%) with the molar ratios of 80 : 20 were put into the zirconia vessel (30 ml internal volume) with ten pieces of zirconia balls. Then, the mixture was mechanically milled for 20 h at 370 rpm under 0.1 MPa of argon gas atmosphere using a planetary ball milling apparatus (Fritsch P7). The samples before and after ball milling were always handled in a glove-box filled with a purified Ar gas atmosphere (Miwa MFG). The catalyzed MgH₂

containing 1 mol% Nb₂O₅ (Sigma Aldrich, 99.5%) and 99mol% of MgH₂ (Alfa Aesar, 98%) is synthesized by ball-milling for 20h. The anode materials of pristine MgH₂ and catalyzed MgH₂, solid electrolyte 80Li₂S-20P₂S₅, and acetylene black were mixed with moderate weight ratios. These mixtures were ground and then pressed into 16 mm diameter tablet. The solid electrolyte 80Li₂S-P₂S₅ was also pressed into 16 mm diameter tablet. Then, these tablets of the pristine MgH₂/catalyzed MgH₂ anode and 80Li₂S-P₂S₅ solid electrolyte were placed on a lithium metallic disk in the experimental cell (Toyo System Co.). The anode properties of pristine /catalyzed MgH₂ were examined as a cathode against counter electrode of lithium metal. All the procedures were done in the Ar glove box.

The charge and discharge properties were measured by galvanostat (HJ-SM8, Hokuto Denko Co.) at a voltage between 0.1V and 2.3V versus Li⁺/Li, current density of 0.05 mA cm⁻², temperature of 100 °C and current density 0.005 mA cm⁻², temperature of 25 °C. The structural characterization was examined by X-ray diffraction measurement (Rigaku, RINT2500) using Cu K α radiation at room temperature. The samples were protected with polyimide film to avoid the oxidation and the adsorption of water during XRD measurement.