Supplementary Information

Totally Atom-Economical Synthesis of Nano/Micro-Structured Nickel

Hydroxide Realized by an Ni-O₂ Fuel Cell

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1. Calculation for atom economy

(1) The conventional process

Atom economy is defined as a measure of the proportion of reactant atoms which are incorporated into the desired product of a chemical reaction. It can be calculated by the equation below.^[1]

Atom economy = (mass or molecular weight of the desired product(s) \div mass or molecular weight of all reactants) \times 100%

The calculation for atom economies of the reactions in Schematic 1a is as follows.

A1: $Ni + H_2SO_4 + 2HNO_3 = NiSO_4 + 2NO_2 + 2H_2O$

Atom economy = molecular weight of NiSO₄ \div (molecular weight of Ni + molecular weight of H₂SO₄ + 2 × molecular weight of HNO₃) × 100% = (58.7 + 32.1 + 16 × 4) \div (58.7 + (2 + 32.1 + 16 × 4) + 2 × (1 + 14 + 3 × 16)) × 100% = 154.8 \div 282.8 × 100% = 54.7%

A2: $NiSO_4 + 2NaOH = Ni(OH)_2 + Na_2SO_4$

Atom economy = molecular weight of Ni(OH)₂ \div (molecular weight of NiSO₄ + 2 \times

molecular weight of NaOH) × 100% = $(58.7 + 17 \times 2) \div (58.7 + 32.1 + 20.1)$

$$16 \times 4 + 2 \times (23 + 17) \times 100\% = 92.7 \div 234.8 \times 100\% = 39.5\%$$

Atom economy of the route = $54.7\% \times 39.5\% = 21.6\%$

(2) The proposed process by a nickel-oxygen (Ni-O₂) fuel cell

 $Ni + 1/2O_2 + H_2O = Ni(OH)_2$

Atom economy of the rout = molecular weight of Ni(OH)₂ ÷ (molecular weight of Ni + 1/2 × molecular weight of O₂ + molecular weight of H₂O) × 100% = $(58.7 + 17 \times 2) \div (58.7 + 1/2 \times 16 \times 2 + 18) \times 100\% = 92.7 \div 92.7 \times 100\% = 100\%$

Supplementary Figures

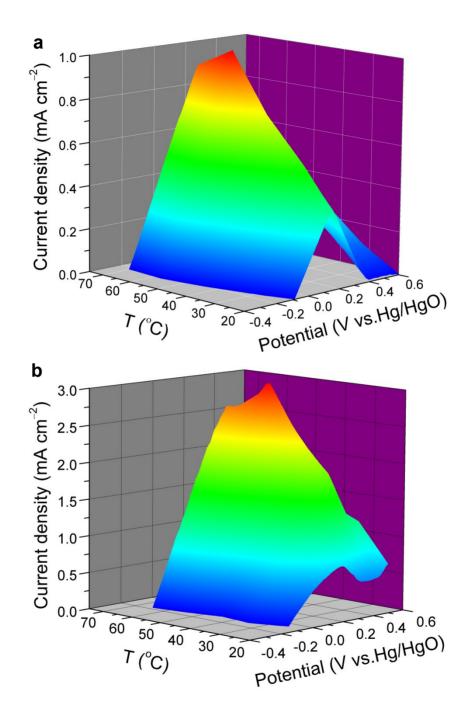


Fig. S1 Anodic polarization curves of (a) an Ni plate anode and (b) an Ni foam anode against temperature. An Ni anode, an Ni wire, and an Hg/HgO electrode were, respectively, used as the working electrode, the counter electrode, and the reference electrode. The electrolyte was a

mixture of 0.50 mol L⁻¹ Na₂SO₄ and 1.0 mol L⁻¹ NH₃·H₂O. Its pH was adjusted by NaOH in the range of 11.30–11.50. The potential scanning rate was 2 mV s⁻¹ in the range of -0.3 to 0.6 V.

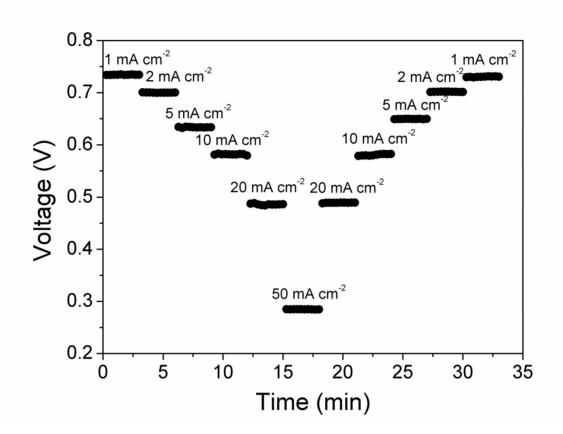


Fig. S2 Stability testing of the Ni–O₂ fuel cell with an Ni foam anode. The fuel cell operated galvanostatically in an aqueous electrolyte of 0.50 mol L^{-1} Na₂SO₄, 2.0 mol L^{-1} NH₃·H₂O, and 0.60 mol L^{-1} NaCl at 55 °C.

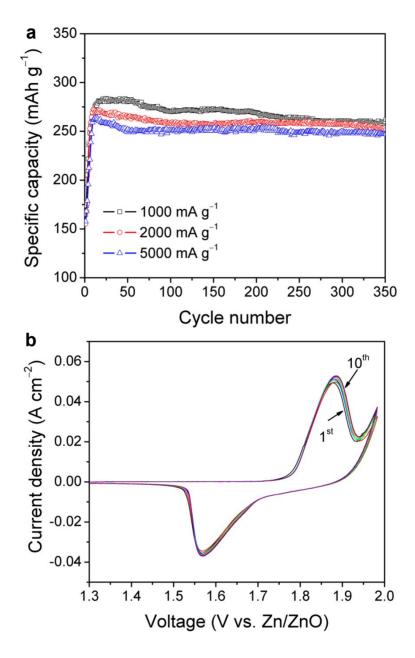


Fig. S3 (a) Cycle curves at three different discharge current densities and (b) first 10 cycles of the cyclic voltammograms of the synthesized nano/micro structured β -Ni(OH)₂ samples at potential scanning rate of 1 mV S⁻¹. The experiments were carried out with a three-electrode configuration (β -Ni(OH)₂ working electrode, Zn/ZnO reference electrode, and Ni wire counter electrode) in a 6.0 mol L⁻¹ KOH aqueous solution.

References:

[1] B. Trost, *Science* 1991, *254*, 1471-1477.