

# Fuel Cell Research Based on Electrochemical Analysis

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**Abstract:** With the development of social economy and the improvement of people's living level, the global energy demand is rising rapidly. The reserves of traditional fossil energy such as coal, oil and natural gas are limited, and its depletion is inevitable. And the massive use of fossil energy will also bring a series of environmental problems such as greenhouse effect. Therefore, it is urgent to find a clean and renewable energy. Fuel cell (FC) is a new energy technology that has attracted much attention. It is a power generation system that converts the chemical energy of fossil fuel (coal, oil, natural gas, etc.), biomass fuel or other hydrocarbon fuel (ethanol, propane, butane, etc.) into electrical energy directly without combustion through electrochemical reaction. In the process of fuel cell operation, fuel and air react in different chambers respectively, breaking away from the restriction of Carnot cycle. In this way, the utilization rate of fuel has been greatly improved. Moreover, the fuel cell will only produce  $H_2O$ ,  $CO_2$  and other products in the working process, and will not produce dust or other harmful gases. Therefore, the research and development of efficient and clean new energy technology is of great significance to promote the rational use of coal resources and biomass fuel and coordinate the harmonious development of environment and economy.

**Keywords:** Electrochemical analysis; Clean energy; Fuel cell

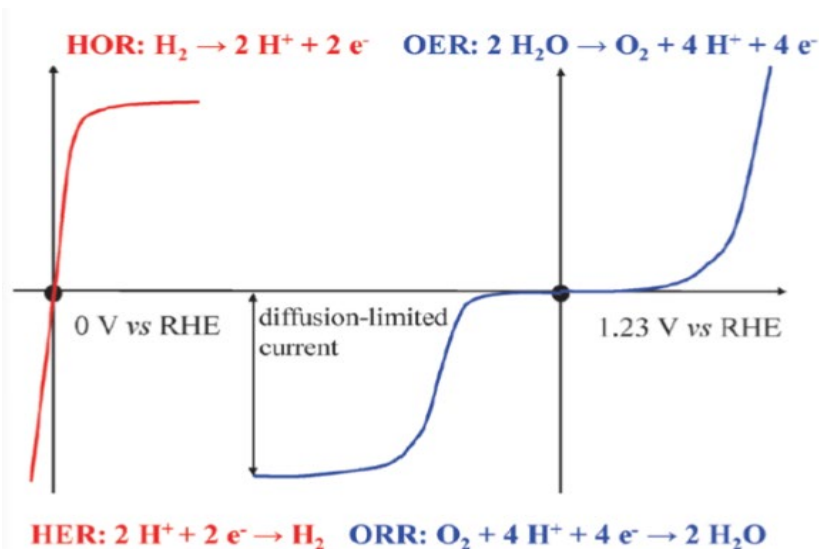
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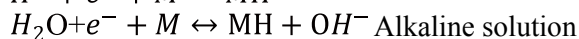
## 1 Electrochemical reaction analysis of hydrogen evolution reaction

Hydrogen is a high-energy density, zero-carbon emission, clean and renewable energy. However, the effective preparation of hydrogen is always a big problem. At present, it is considered to be a very effective means through the electrolysis of water to produce hydrogen, with the use of solar energy, wind energy, geothermal energy, tidal energy and other new energy generating the surplus electric energy. In the preparation of hydrogen and the utilization of hydrogen energy, four important electrochemical reactions are inevitably involved, namely, the hydrogen evolution reaction in the hydrogen production process of electrolytic water, as shown in Figure 1. For the hydrogen evolution reaction, it must include the electrochemical adsorption step (Volmer reaction) and at least one desorption step, see the formula (1-3). The desorption reaction mainly depends on the nature of catalyst. In a certain range of the overpotential, the overpotential  $\eta$  and current density  $i$  of the hydrogen evolution reaction meet the Tafel equation, that is,  $\eta = a + b \lg i$ , where  $b$  is the Tafel slope. For different reaction paths, the Tafel slope has different values, so the Tafel slope can be used to determine the mechanism of hydrogen evolution reaction.



**Figure 1.** polarization curves of two groups of extremely important electrochemical reactions in the field of energy catalysis, namely, hydrogen oxidation reaction (HOR) and hydrogen evolution reaction (HER), oxygen evolution reaction (OER) and oxygen reduction reaction (ORR)<sup>[1]</sup>.

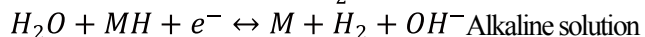
(1) Electrochemical step (Volmer reaction)



(2) Composite desorption step (Tafel reaction)



(3) Electrochemical desorption step (Heyrovsky reaction)



## 2 Synthetic analyses of catalytic materials for hydrogen evolution reaction

### 2.1 Alloy electrode materials of transition element metals

Looking for active hydrogen cathode materials: (1) using noble metals directly; (2) using nickel-based materials, including nickel metals, nickel-based alloys, nickel-based composite materials, porous nickel, etc. Once a large number of literatures reported that noble metal Pt group elements have excellent electro-catalytic activity, and their hydrogen Superpotential is low, but noble metals are expensive and cannot be used in large quantities. Therefore, many researchers are committed to the research of nickel-based materials.

### 2.2 Electrode materials of composite alloy coating

Composite alloy coating is obtained by adopting composite electro-deposition. The so-called composite alloy coating refers to the formation of composite alloy

layer by embedding the second phase solid particles in the base metal (such as Ni), which is a new method to prepare high catalytic active electrode materials.

### 2.3 Amorphous alloy electrode materials

The composition of the alloy is changed in a large range to achieve the required electronic structure and form the best electro-catalytic activity. The catalytic activity centers are uniformly distributed on the surface in a single form (Solid solution).

### 2.4 Alloy electrode materials of rare-earth elements

Ni-La alloy is prepared by electro-deposition from aqueous solution. The activity of hydrogen evolution in 25% NaOH solution is much higher than that of Ni electrode. Ni-Mo alloy and rare-earth hydrogen storage alloy are alternately plated on the electrode surface to form a catalytic layer for hydrogen evolution reaction by adopting alloy electro-deposition and composite plating. The introduction of rare-earth hydrogen storage elements not only improves the catalytic activity of the electrode for hydrogen evolution reaction, but also enhances the oxidation resistance of the catalytic layer, thus prolonging the service life of the electrode<sup>[2]</sup>.

### 2.5 Nano-alloy electrode materials

By electro-deposition, pure metals, alloys and metal-ceramic composites with nanostructures can be prepared economically and simply. So it has a good application

prospect in electro-catalysis and hydrogen storage.

### 3 Strategies to improve electro-catalytic properties of materials

#### 3.1 Increase the number of active sites

Molybdenum disulfide is a kind of layered material. However, there is no catalytic activity in the layer plane, and the catalytic active sites of hydrogen evolution reaction are mainly concentrated at the edge of the layered structure. Therefore, the increase of the number of active sites needs to optimize the ratio of edge to base plane. Such methods mainly include the nanostructure and the introduction of defects or porous structures in the lamellar structure. In 2013, Kong *et al.* reported the synthesis of molybdenum disulfide nano-flakes perpendicular to the substrate. The upper surface of this material is completely composed of molybdenum disulfide edges. Therefore, it shows excellent catalytic activity of hydrogen evolution. In 2015, Guo *et al.* reported the growth of molybdenum disulfide nanoparticles on carbon nano-fibers<sup>[3]</sup>. Its small size and uniform distribution ensure the exposure of more active sites, and obtain better hydrogen evolution catalytic activity. Wang *et al.* in this group prepared molybdenum disulfide nanoparticles with different sizes by ultrasonic and gradient centrifugation, and studied the size effects of hydrogen evolution and oxygen reduction electro-catalysis. The experimental results show that the smaller the size of molybdenum disulfide

nanoparticles, the stronger the ability of catalyzing hydrogen evolution and oxygen reduction, and the best catalytic performance is obtained for molybdenum disulfide nanoparticles with a particle diameter of about 1.5 ~ 2nm. This is further confirmed by the work of Benson *et al.*

#### 3.2 Enhanced conductivity

The electro-catalytic properties of the materials are directly related to their conductivity. The materials with high conductivity can transfer electrons faster. This requires not only good catalytic activity for electro-catalytic materials, but also good contact between materials and substrate. In 2011, Li *et al.* reported the synthesis of molybdenum disulfide nanoparticles and reduced graphene oxide composite, and this MoS<sub>2</sub>/RGO composite has good catalytic activity and stability for hydrogen evolution<sup>[4]</sup>. In this work, graphene provides good conductivity, and highly-dispersed MoS<sub>2</sub> nanoparticles can be obtained in the presence of graphene. By using LPCVD method, Shi *et al.* grew monolayer MoS<sub>2</sub> on gold foil, and the electronic coupling between molybdenum disulfide and gold foil ensured good conductivity and obtained better catalytic activity. In 2016, through experiments Voiry *et al.* proved that the catalytic activity of substrate plane of molybdenum disulfide 2H phase could even be enhanced by using the electronic coupling between gold substrate and MoS<sub>2</sub>. (As shown in Figure 2.)

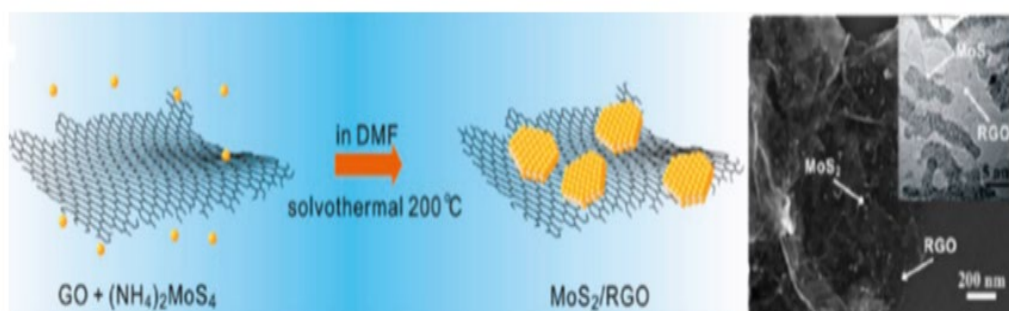


Figure 2. Diagram of MoS<sub>2</sub>/RGO composite material synthesis

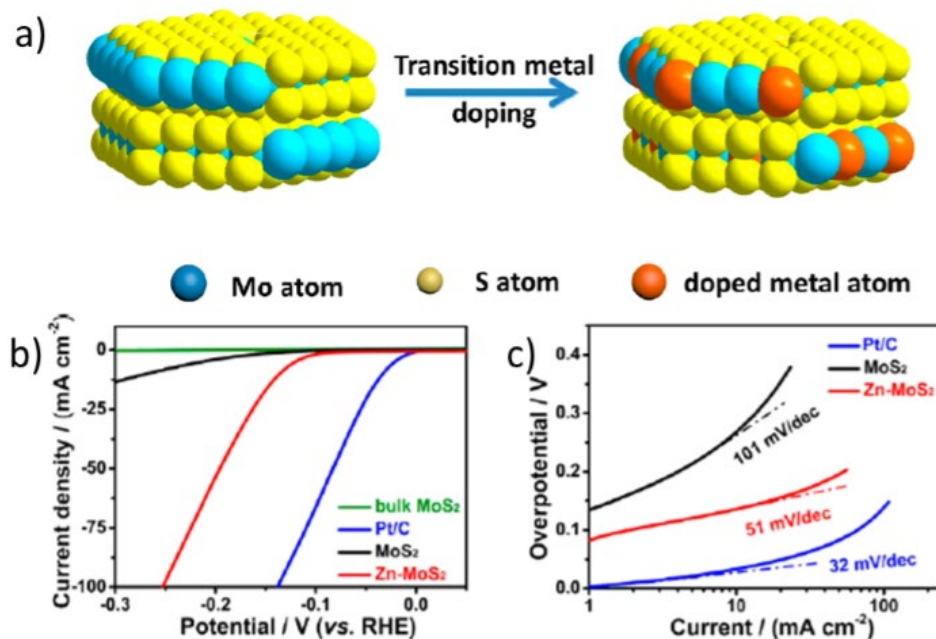
#### 3.3 Improving the catalytic activity of the material itself

The improvement of the intrinsic catalytic performance for materials is also an important means to enhance the catalytic activity. Its main ideas include doping other atoms and structure optimization. In 2015, through theoretical calculation and experiments Wang *et al.*

showed that doping transition metal atoms such as Fe, Co, Ni and Cu in the structure of molybdenum disulfide could adjust the electronic state and hydrogen-adsorption free energy of molybdenum disulfide, thus improving the catalytic activity of hydrogen evolution reaction of the material. In 2017, Shi *et al.* reported that (NH<sub>4</sub>)<sub>2</sub>MoS<sub>4</sub> and Zn(NO<sub>3</sub>)<sub>2</sub> were used as precursors to

prepare Zn modified molybdenum disulfide nanoflakes by hydrothermal method. This composite material has better catalytic activity for hydrogen evolution reaction. In addition, Yuwen *et al.*<sup>[5]</sup> reported that the synergistic effect between MoS<sub>2</sub> and Pd and other noble metal atoms could improve the catalytic effect on methanol oxidation; Li *et al.* showed that the catalytic effect on hydrogen peroxide reduction could be improved

by modifying Au-Pd bimetallic nanoparticles on molybdenum disulfide nanoflakes. In 2013, Lukowski *et al.* obtained 1T-phase MoS<sub>2</sub> by stripping 2H-phase MoS<sub>2</sub> with the method of lithium ion insertion. 1T-phase MoS<sub>2</sub> is one kind of metallic-state material. And its catalytic activity of hydrogen evolution is better than that of 2H-phase MoS<sub>2</sub> with semiconductor properties. (As shown in Figure 3.)



**Figure 3.** (a) Schematic diagram of doping other transition metal atoms on molybdenum disulfide material; the polarization curve (b) and Tafel curve (c) of Zn-MoS<sub>2</sub> catalyst for hydrogen evolution and the comparison with other catalysts.

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