Development of CoCuFeNiMnMox (x= 0.5, 1, and 1.5) High-Entropy Alloy Electrocatalysts for Water-Splitting Applications via Mechanical Alloying and Spark Plasma Sintering

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This study explores the influence of Mo ratio on the electrocatalytic properties of $CoCuFeNiMnMo_x$ (0.5, 1.0, and 1.5) high-entropy alloys (HEAs) for water-splitting applications. The structural and electrochemical characteristics of these alloys were systematically investigated to elucidate the relationship between Mo content and catalytic performance. X-ray diffraction (XRD) analysis revealed the presence of both face-centered cubic (FCC) and body-centered cubic (BCC) phases in all samples. Rietveld analysis of the XRD patterns indicated a decreasing trend in the BCC phase content and an increasing trend in the FCC phase content with decreasing Mo ratio.

Microstructural analysis confirmed the preservation of a porous structure across all Mo ratios, with consistent phase distributions. Hardness measurements revealed that the $NiCoCuFeMnMo_{0.5}$ alloy exhibited the highest hardness among the tested compositions. Furthermore, linear sweep voltammetry experiments were conducted to assess the electrocatalytic activity of the alloys for the oxygen evolution reaction (OER) and the hydrogen evolution reaction (HER).

Remarkably, the results demonstrated that the sample with the lowest Mo ratio exhibited the highest electrocatalytic activity for both OER and HER. Specifically, the $NiCoCuFeMnMo_{1.5}$ alloy exhibited superior HER performance, while the $NiCoCuFeMnMo_{0.5}$ alloy showed exceptional OER activity. These findings highlight the significance of Mo ratio optimization in tailoring the catalytic properties of HEAs for water-splitting applications.

Overall, this investigation sheds light on the relationship between Mo ratio and electrocatalytic performance in $CoCuFeNiMnMo_x$ high-entropy alloys, providing valuable insights for the design and development of efficient electrocatalysts for sustainable energy conversion processes.