

## High Entropy Alloy Nanoparticles as OER catalyst for Green Hydrogen

### Abstract

In this App Note we present data for high entropy alloy nanoparticles generated using gas phase synthesis. We will show how these materials can be used as cheap and efficient electrocatalysts for Oxygen Evolution Reaction to generate of green hydrogen through water splitting.

### Introduction

The drive to achieve net zero carbon emission by 2050 has highlighted the need for improvements to current green technologies, including methods for generating green hydrogen. Water electrolysis is widely accepted as the greenest method for producing hydrogen. However, one of the barriers to the scale up of this technology is the high cost and scarcity of the platinum group metals which are currently used as electrocatalysts for reactions at both the cathode and anode. High Entropy alloys (HEAs) offer an earth abundant and cheap alternative to Iridium for the Oxygen Evolution Reaction, which occurs at the anode. HEAs are formed from equal parts of five or more elements, such as Al, Fe, Co, Mo, Ni, Zr, Ti and Cr, and offer tuneable activity combined with excellent thermal and chemical stability.



Nikalyte have teamed up with the Rob Weatherup group at Oxford University, on a Henry Royce Institute funded project, to generate high purity HEA nanoparticles using Nikalyte gas phase synthesis technology. The nanoparticles were produced from a single alloy target using the NL-UHV nanoparticle source (shown in Fig 1). The electrocatalysts were analysed using EDS, HRTEM to ascertain the material composition and nanoparticle size. The electrochemical performance of the material was then assessed in a OER electrolyser half-cell.

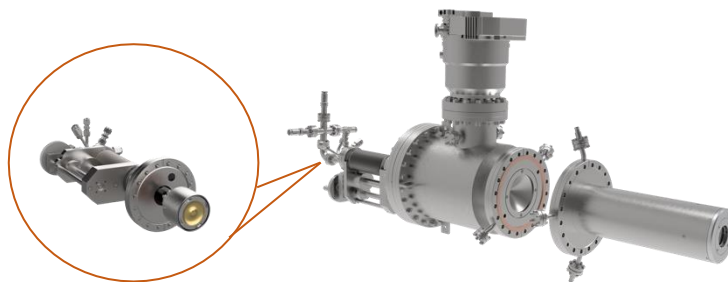


Figure 1 NL-UHV nanoparticle source with NL-QMS mass filter and 2inch sputter source (circled).

### Experimental Conditions

In this experiment alloy nanoparticles were generated from 2-inch alloy targets of NiCoFeMoCr and NiCoFeMoAl, using argon sputter gas and a pulsed dc power supply. The pulse width and duty cycle were optimized to provide a stable deposition rate of 5-10ng/cm<sup>2</sup>/s. Nanoparticles were deposited on glassy carbon discs, TEM grids and silicon substrates.

### Microscopy Results

Figure 2 shows the HRTEM of NiFeCoMoCr and NiFeCoMoAl nanoparticles, measured by the Weatherup Group. The nanoparticles have a narrow size distribution between 5nm and 8nm and have self-organized into chains to align the magnetic dipoles. The EDS elemental maps of the NiFeCoMoCr nanoparticles confirm the presence five-element alloy nanoparticles.

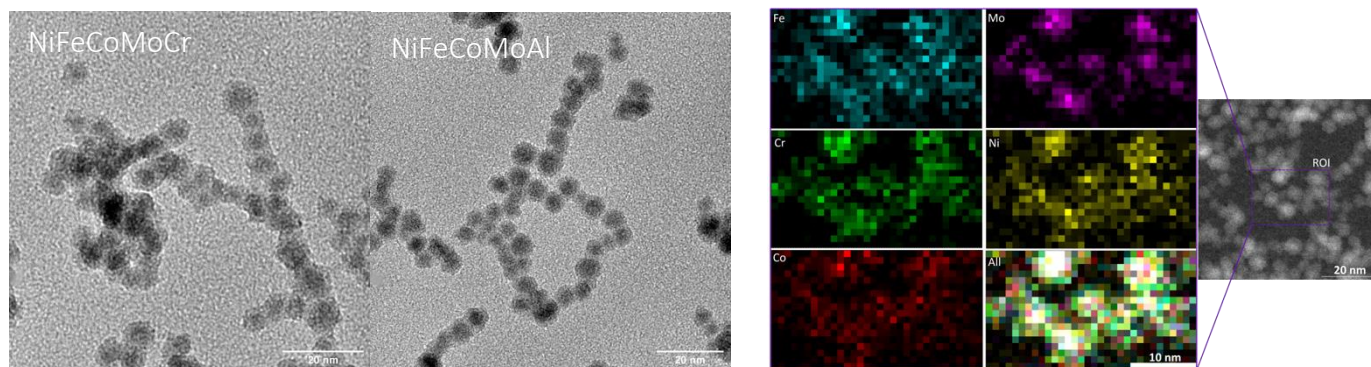


Figure 2 HRTEM images of NiFeCoMoCr (left) and NiFeCoMoAl (centre) nanoparticles, EDS elemental map of NiFeCoMoCr nanoparticles (right). Credit: Leanne Jone, Peixi Cong, Longxiang Liu, University of Oxford.

## Electrochemical Results:

The electrochemical performance of the two different HEA nanoparticle samples deposited onto glassy carbon was compared with elemental Ni nanoparticles using a half-cell, with 1Molar KOH electrolyte, Pt control electrode and Hg:HgO reference electrode. The cyclic voltammetry sweeps for both HEAs and pure Ni nanoparticles are plotted in Figure 3. All plots show distinct oxidation and reduction peaks, which are different from the pure Ni catalyst experiment, confirming that the elements other than the Ni is active in these alloy catalysts. The over potentials are comparable with the Ni. Figure 3 also shows the Tafel plots for the HEA nanoparticles and the Ni nanoparticles. The Tafel slope gives information about the activation energy of the Oxygen evolution reaction and the higher slope measured for the HEA nanoparticles compared to the Ni nanoparticles indicates that the alloy catalyst materials are less efficient than elemental Ni. However, there are some significant differences in the size of the nanoparticles and improvements to the experiment are required to provide more conclusive comparison of performance.

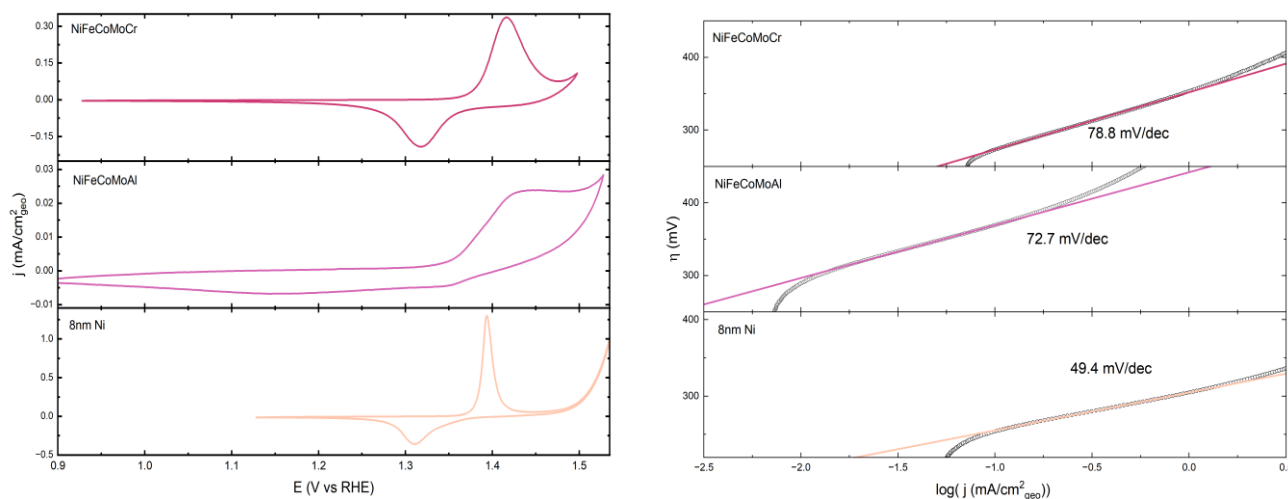


Figure 3 CV sweeps (left) and Tafel analysis (right) for the HEA and Ni nanoparticles. Credit: Leanne Jones, University of Oxford.

## Conclusions:

This work has shown that High Entropy alloy nanoparticle with different alloy compositions can be generated using gas phase synthesis. The electrochemical performance of high entropy alloy nanoparticles as an oxygen evolution reaction catalyst has shown very promising overpotentials and reactivities and proved that these materials merit further investigation as a potential replacement to Iridium to produce green hydrogen.