Catalyzing a Green Hydrogen Future: Investigating Iron-Nickel Borides as Nanocatalysts for Water Electrolysis

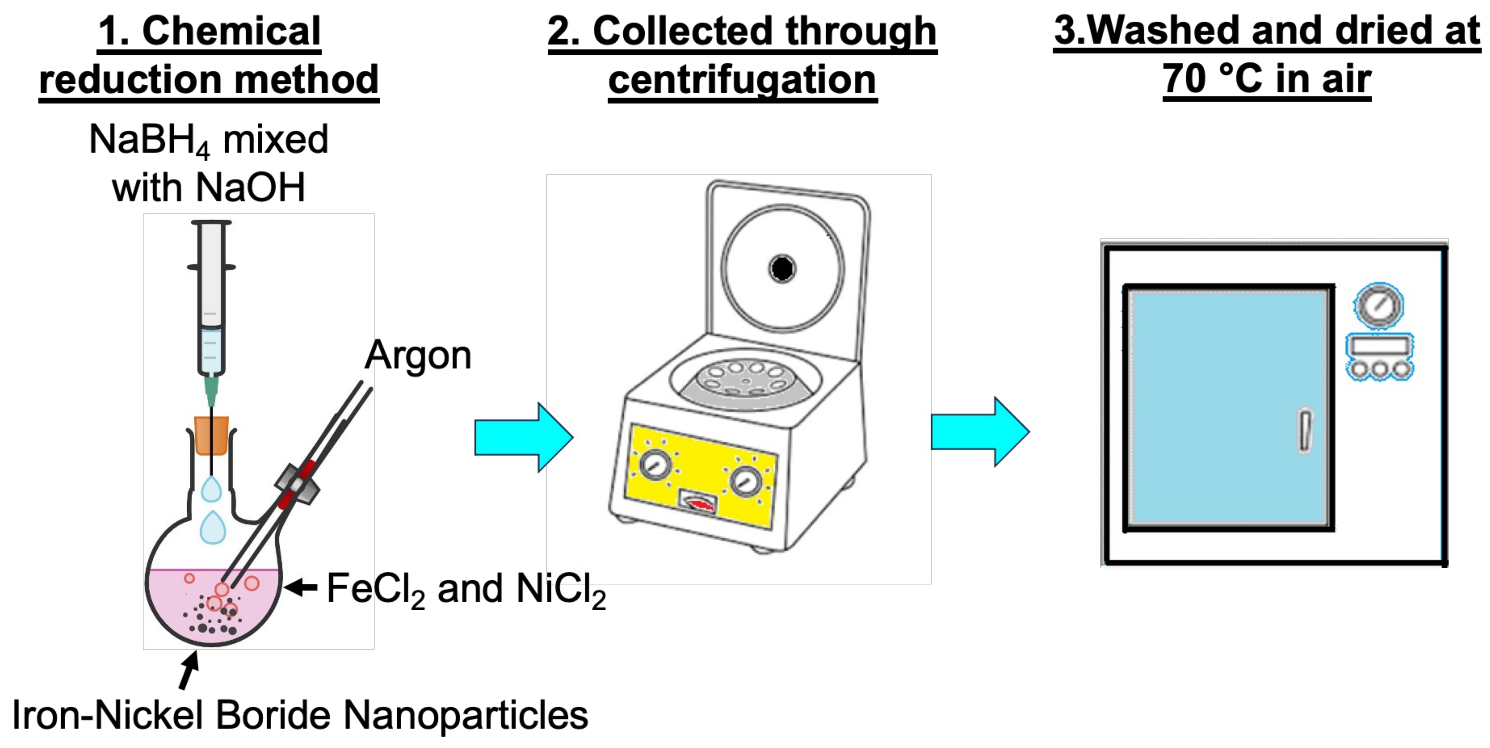
Bennett Schmitt and Dr. Veronica Sofianos

Introduction

Hydrogen offers robust potential as an energy carrier, but it is primarily produced as a derivative of fossil fuels. Avenues for producing hydrogen from water and renewable energy systems are critical for a future powered by decarbonized energy. Water electrolysis—the process by which electricity is used to split water to O_2 and H_2 gas—stands as the most promising green hydrogen production strategy for its ability to draw on carbon-free renewable energy sources. Metal borides exhibit immense potential as cost-effective nanocatalysts for electrochemical water splitting reactions due to their relative abundance in Earth's crust, high conductivity, advantageous thermal stability, and catalytic activity. This work investigates the synthesis and characterization of iron nickel borides and explores their capacity as electrocatalysts for hydrogen and oxygen evolution reactions in green hydrogen production.

Methodology

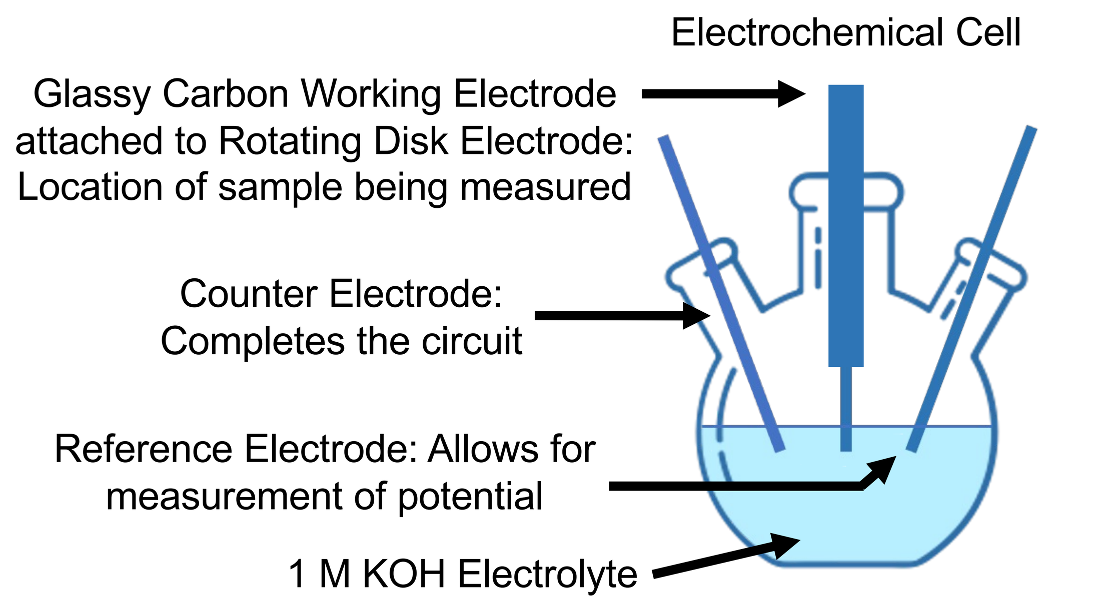
Synthesis of Iron-Nickel Boride Nanoparticles



Fe to Ni molar ratio	Sample Name
0.9/1	FeNiB-I
1/1	FeNiB-II
1/0.9	FeNiB-III

Table 1. Sample naming scheme for synthesized FeNiB nanocatalysts determined by iron/nickel molar ratio.

Electrochemical Analysis



- Electrochemical cell helps investigate the movement of electrons in the oxygen evolution reactions (OER) and hydrogen evolution reactions (HER)
- Linear sweep voltammetry (LSV) allows for the sweeping of potential across the cell and measure of its current response

Results

Powder X-Ray Diffraction

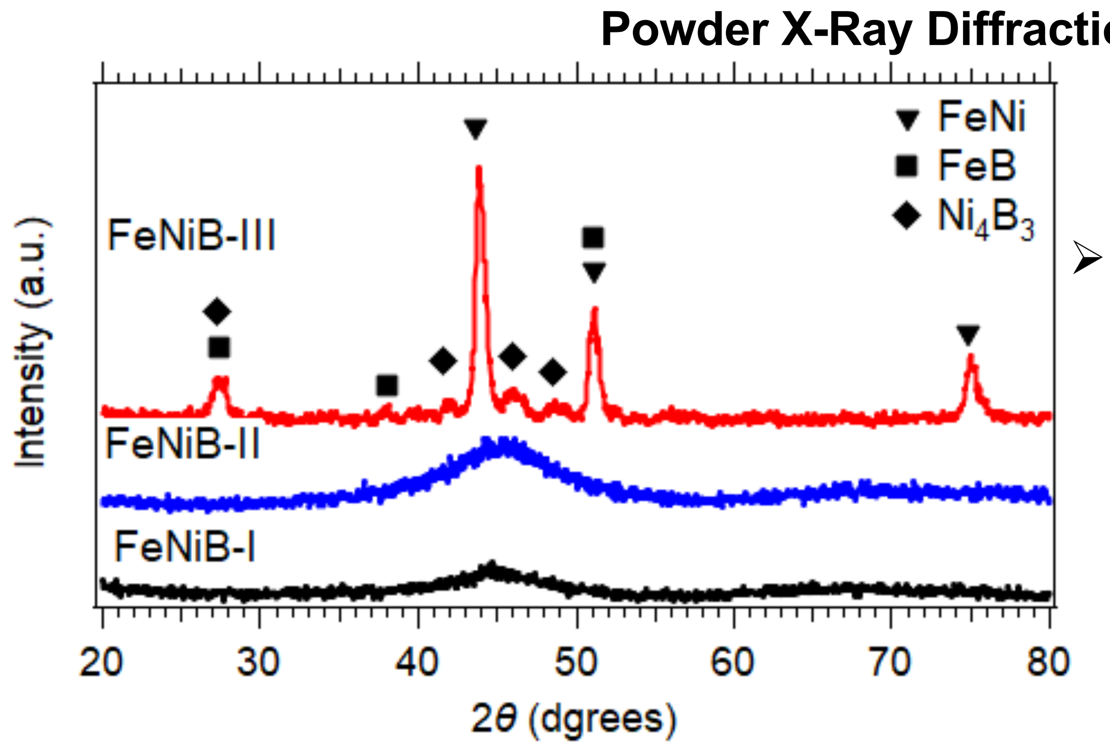


Figure 1. Powder XRD patterns for FeNiB nanocatalysts with phases identified.

- FeNiB-I and II exhibited a broad Bragg diffraction peak between 40° and 50° assigned to the Fe-Ni-B amorphous phase.[2] Fe-NiB-III showed defined diffraction peaks of the FeNi, FeB, and Ni_4B_3 phase

Proposed Reduction Schemes

$$FeCl_2 + NiCl_2 + 4NaBH_4 + 9H_2O \rightarrow FeNiB + 4NaCl + 12.5H_2 + 3B(OH)_3 \quad (1)$$

$$FeCl_2 + 2NaBH_4 + 6H_2O \rightarrow FeB + 2NaCl + 10H_2 + 2B(OH)_3 \quad (2)$$

$$4NiCl_2 + 8NaBH_4 + 15H_2O \rightarrow Ni_4B_3 + 8NaCl + 23.5H_2 + 5B(OH)_3 \quad (3)$$

Morphological Observations

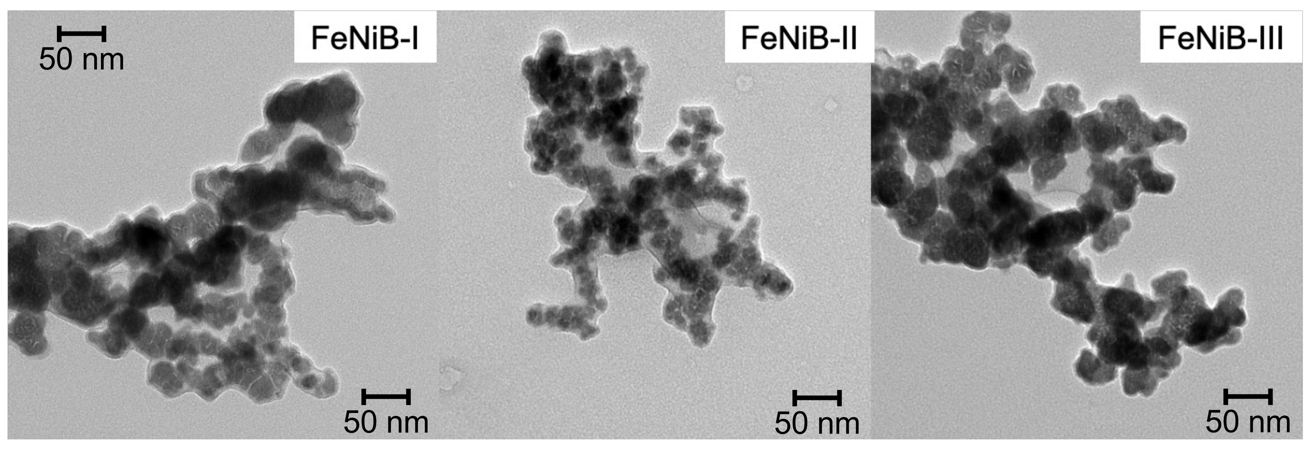


Figure 2. Transmission Electron Microscopy (TEM) micrographs for FeNiB samples.

Electrocatalysis

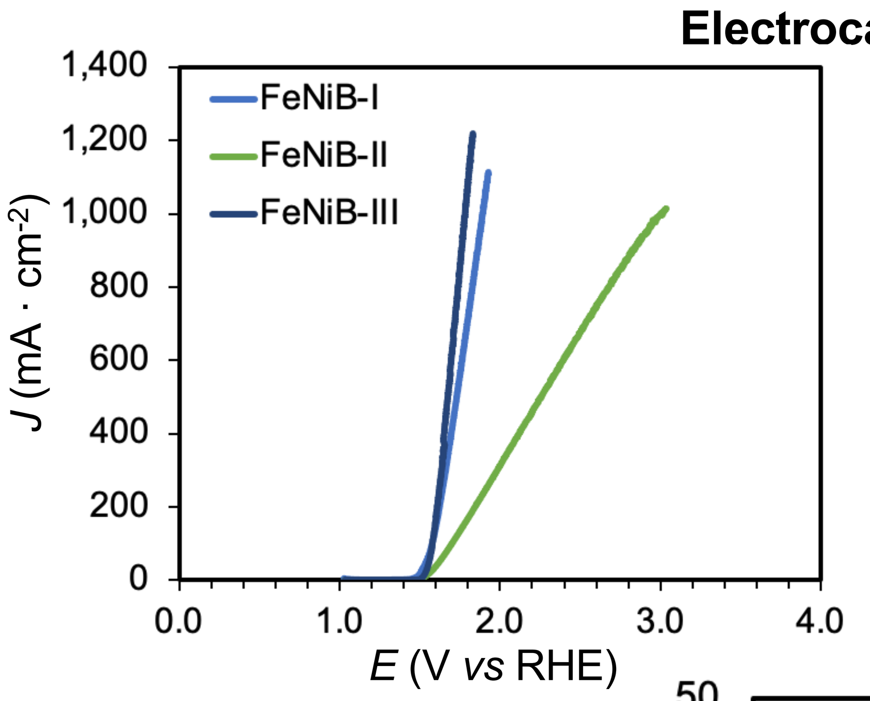


Figure 3. Current density (J) vs. potential (E) linear polarization curves obtained from oxygen evolution linear sweep voltammetry in pH 14 electrolyte.

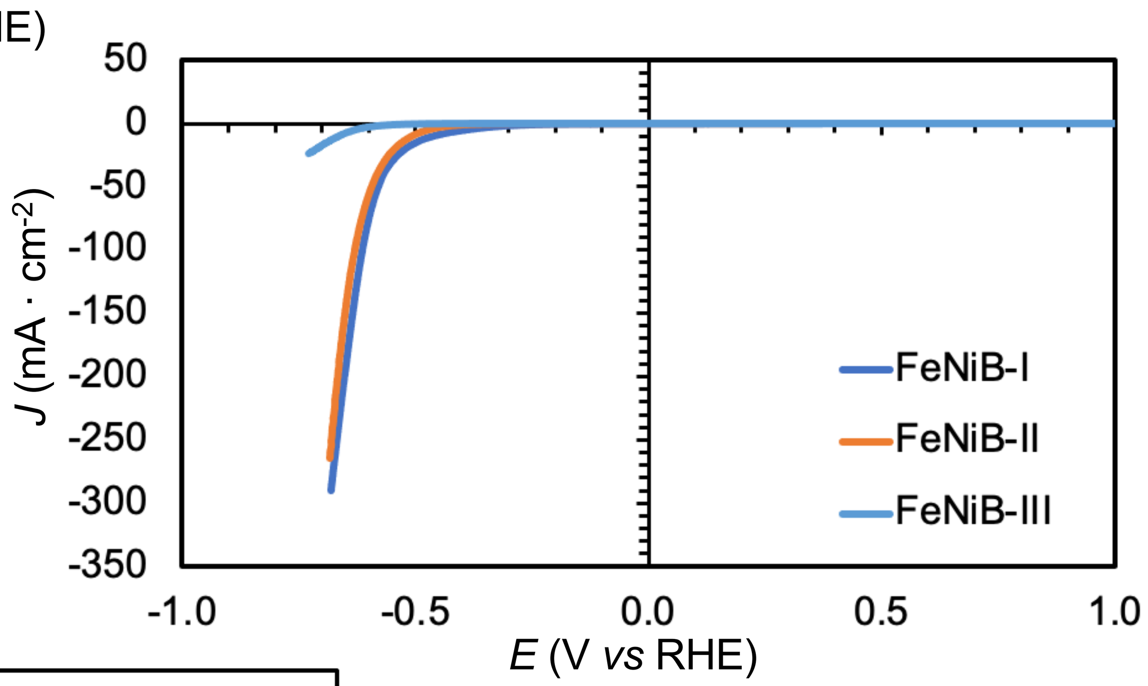


Figure 4. Current density (J) vs. potential (E) linear polarization curves obtained from hydrogen evolution linear sweep voltammetry in pH 14 electrolyte.

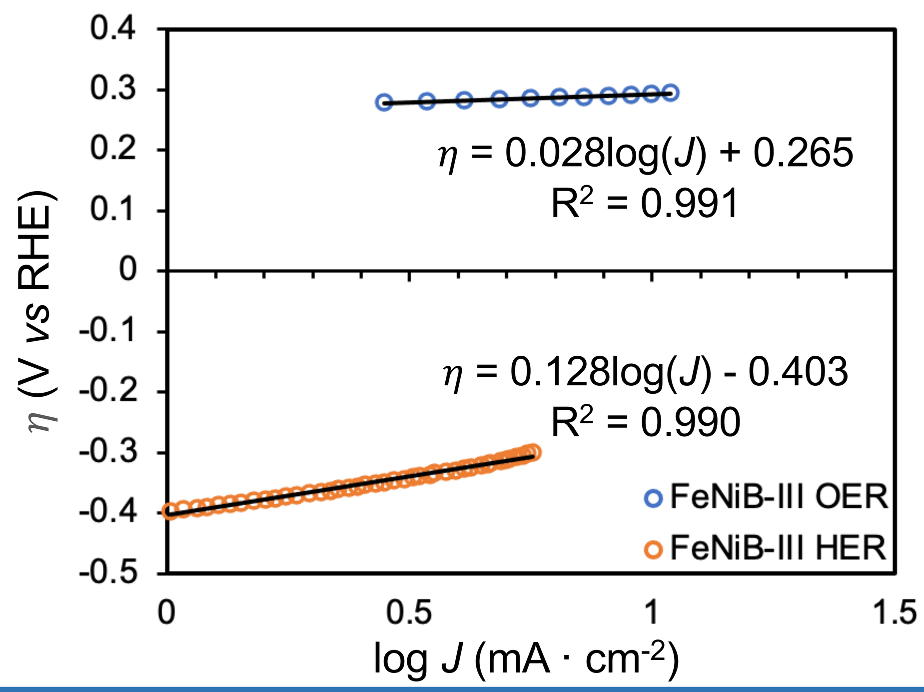


Figure 5. OER and HER Tafel plots of samples in pH 14 electrolyte derived from the linear polarization curves. Black lines represent the linear regressions, and linear fit equations are shown.

Conclusions

- A simple, one-pot reduction method can be used to synthesise iron-nickel boride nanoparticles of different iron/nickel molar ratios
- Synthesised FeNiB nanoparticles show varying degrees of crystallinity depending on iron/nickel molar ratios. As Fe concentration increases, crystallinity of the sample also increases
- The FeNiB nanoparticles in all three samples exhibit a flaky morphology and are polydisperse in size
- Iron/nickel molar ratios influence performance of the metal boride in oxygen and hydrogen evolution reactions:
  - Sample FeNiB-III exhibits the greatest current density in the OER
  - Sample FeNiB-I exhibits the greatest current density in the HER
- FeNiB-III produced the smallest Tafel slopes for both OER and HER and thus the highest kinetics

References and Acknowledgements

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2. Yuan, W.; Zhao, X.; Hao, W.; Li, J.; Wang, L.; Ma, X.; Guo, Y., Performance of Surface-Oxidized Ni3B, Ni2B, and NiB2 Electrocatalysts for Overall Water Splitting. *ChemElectroChem* **2019**, *6* (3), 764-770 DOI: https://doi.org/10.1002/celc.201801354.

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