

Material Development for Electro-Catalysis and System-Level Integration for Future Hybrid Energy Systems



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for the Award of degree**

Doctor of Philosophy

By

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Chapter 8

Major Conclusions and Scope for Future Work

8.1. Major conclusions of the present work

The global shift toward sustainable, low-carbon energy systems demands technologies that are efficient, clean, and capable of decentralized operation. Fossil fuel-based power generation remains a leading source of greenhouse gas emissions, highlighting the need for viable alternatives. Renewable energy sources, particularly solar photovoltaics combined with electrochemical energy conversion technologies such as fuel cells and hydrogen generation, offer a promising pathway toward a clean, reliable, and flexible energy supply. Their integration addresses intermittency challenges, enhances energy security, and supports the broader objectives of de-carbonization and long-term sustainability.

Building on this vision, the present thesis explored the design, development, and evaluation of advanced renewable and electrochemical energy systems. Through systematic investigation ranging from material synthesis and performance characterization to system-level engineering, this work addresses key challenges in enhancing efficiency, durability, and scalability. To achieve this objective, the present work advances the development of materials for electrocatalysis in the oxygen evolution reaction (OER) for hydrogen generation and the methanol oxidation reaction (MOR) in direct methanol fuel cells.

Our first study demonstrates that $(\text{Ni}_{187}\text{Fe}_4\text{Cr}_9)_{78}\text{Si}_8\text{B}_{14}$ amorphous ribbons, when subjected to controlled potentiostatic cathodic corrosion, can be effectively transformed

into high-performance, self-supported electrocatalysts for both the oxygen evolution reaction (OER) and the methanol oxidation reaction (MOR). The surface modification process induces the formation of densely distributed nano-sized (5–10 nm) α -Ni(OH)₂ particles, with optimal nanocrystallization observed between 45 and 90 minutes of treatment. Among the tested conditions, the 60-minute treated ribbon (S60) achieved the best OER activity in 1 M KOH, delivering an over-potential of 295 mV at 10 mA cm⁻² and a Tafel slope of 51 mV dec⁻¹, while the 90-minute treated ribbon (S90) exhibited the most efficient MOR performance in 1 M KOH + 1 M MeOH, requiring only 1.38 V vs. RHE at 10 mA cm⁻² with a Tafel slope of 34 mV dec⁻¹. The addition of methanol notably reduced the anodic potential compared to OER, indicating a substitution effect that enhances energy-efficient hydrogen generation at the cathode. The improved electrocatalytic performance is attributed to the formation of Ni(OH)₂ or NiOOH active phases, which facilitate electro-oxidation and reduce charge-transfer resistance. These findings highlight the potential of surface-engineered Ni-based amorphous ribbons as durable, efficient catalysts for sustainable hydrogen production and direct methanol fuel cell applications.

In addition, scalable synthesis of nanoporous (Ni₈₇Fe₄Cr₉)₇₈Si₈B₁₄ amorphous ribbon with active α -Ni(OH)₂ phase for efficient oxygen evolution (OER) and methanol oxidation reaction (MOR) is also reported through surface de-alloying. Surface de-alloying in 0.5 M HNO₃ for 60 minutes generates a dense, ~2 μ m-thick (NiCr) oxy/hydroxide network with a nanoporous structure. The resulting electrocatalyst exhibits an overpotential of 290 mV at 10 mA cm⁻², a Tafel slope of 53 mV dec⁻¹, and ECSA of 132 cm² in 1 M KOH. For MOR in 1 M KOH + 1 M MeOH, the treated catalyst demonstrates a low onset potential of 1.35 V vs. RHE at 10 mA cm⁻², with a Tafel slope of 52 mV dec⁻¹ and double-layer capacitance of 66 μ F. This study presents a reproducible

strategy for designing high-performance electrocatalysts for OER and MOR applications. Our findings highlight the scalable synthesis strategy for self-supported electrocatalysts through the surface de-alloying of amorphous alloy ribbon.

The dense network of hydroxide with nano-porous architecture leads to superior OER and MOR performance. The de-alloyed electrocatalyst showed higher ECSA and lower R_{ct} suggesting enrichment of active sites and improved charge transfer kinetics resulting from redistribution of electrons. The present work reports a holistic design for developing noble-metal-free, self-supported and binder-free electro catalysts for cost-effective and scalable energy solutions.

To work towards the PV plant installation, present work also discussed the optimal designing and engineering issues related to supply, installation, testing, and commissioning of 500 kWp OGRTS system installed in the industrial city of Jamshedpur. Critical aspects of project feasibility analysis for defining the electricity utility scenario, shadow analysis, solar radiation analysis, electrical SLD for power distribution along with power evacuation strategies are discussed by correlating the data obtained from the plant site.

In addition, an attempt is made in the form of engineering drawings, flow charts along with techno-economic analysis for a broader insight into the utility and solar sector. Performance parameters of the designed plant, simulated through PVSYST[®] V6.63 is compared with the actual generation data to get the idea of energy output, performance ratio and capacity factors along with techno-economy aspects and life cycle assessment.

8.2. Scope for future work

The present work demonstrates the potential of surface-engineered Ni-based amorphous ribbons as efficient self-supported electrocatalysts for both the oxygen evolution reaction (OER) and methanol oxidation reaction (MOR). However, several research directions can be pursued to further enhance performance, durability, and practical applicability:

Extended Durability Studies: Conduct long-term electrochemical stability tests under realistic operating conditions, including fluctuating temperatures, electrolyte compositions, and cycling loads.

Mechanistic Insights: Utilize advanced in-situ/operando characterization techniques (e.g., in-situ XRD, Raman, XPS, XANES/EXAFS) to elucidate the dynamic phase evolution and identify active sites during OER and MOR.

Composition Optimization: Explore alloying strategies through other Transition elements, incorporating other metals (e.g., Co, Mn, Mo) or non-metal dopants to tune electronic structure and improve catalytic activity.

Surface Engineering Techniques: Investigate alternative or hybrid surface modification methods such as plasma treatment, laser texturing, or chemical etching to enhance active site density and mass transport.

Integration with Device Architectures: Incorporate the optimized ribbons into full fuel cell or electrolyser assemblies to assess system-level performance and compatibility with existing technologies.

Catalyst testing is limited to laboratory-scale electrochemical cells and not full-stack DMFC or water electrolyzer prototypes as it needs full-fledged infrastructure. This work

can be explored. The same methodology can be used on Cathodic side for direct testing of HER.

Experimental testing of full hybrid system integration (PV + fuel cell) is not possible due to infrastructure constraints and left for future scope of work, by using different types of Electrode materials.

Pursuing these directions would deepen understanding of the fundamental mechanisms, improve catalyst design, and accelerate the transition of these materials from laboratory level research to commercial fuel cell and hydrogen generation technologies.