Photoelectrochemical Hydrogen Production

Arun Madan
MVSystems, Inc.
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This presentation does not contain any proprietary or confidential information
Overview

Timeline
• Project start date: TBD
• Project end date: TBD
• 0% complete

Barriers
AP. Materials Efficiency
AQ. Materials Durability
AR. Bulk Materials Synthesis
AS. Device Configuration Design
AT. Systems Design and Evaluation

Budget
• Total project funding: $4,090,172
  – DOE share $3,271,630
  – Cost share $818,542
• Funding received in FY04: $0
• Funding for FY05: $0

Partners
• Hawaii Natural Energy Institute (University of Hawaii)
• Intematix Corporation
• UC Santa Barbara
• Southwest Research Institute
• Duquesne University
• NREL
Objectives

(1) The demonstration of a multi-junction photoelectrochemical solar-powered hydrogen production system with 7.5% solar-to-hydrogen (STH) conversion efficiency and 1,000 hours operational life

- Development of low-cost photoactive materials with 1-sun photocurrents greater than 6 mA/cm² and with sufficient durability to meet the lifetime requirement
- Development of supporting solid-state devices with sufficient current and voltage output
- Development of necessary process integration techniques

(2) The identification of commercialization paths toward DOE plant production cost targets

- Demonstration of materials/device fabrication process scale-up for commercialization
- Generation of an energy/economic analysis for hydrogen production cost based on the developed technology
Approach:

1. Hybrid Photoelectrode Technology*

- Multi-junction monolithic photoelectrode for direct water splitting
- Focus on low-cost materials such as metal foil substrates & oxide thin films
- Utilize scalable fabrication processes for commercial manufacture
- Materials developed for HPE relevant to other multi-junction configurations

*Patented technology developed under DOE Grant DE-FC36-00GO10538 by U. of Hawaii
Approach:
2. Project R&D Task Breakdown

- **Accelerated R&D of Photoactive Materials**
  - High-throughput fabrication and screening of material modifications
  - doping for improved photo-response
  - film texturing for improved surface area
  - Guidance by theoretical calculations…
  - …and detailed analysis of existing high-performance materials

- **Hybrid Photoelectrode (HPE) Device Development**
  - Development of suitable solid-state junctions for device integration
  - Prototype demonstration (several cycles) based on best-available materials

- **Scale-up and Commercialization Evaluation**
  - Medium-scale fabrication of HPE component films on cluster tool
  - Large-scale fabrication of photoactive film (WO$_3$) on vacuum roll system
  - Economic/energy analysis of HPE technology based on current state and projections
Approach:
3. Division of Tasks

MVSystems, Inc.
- Business Management
  Customized a-Si Photovoltaic Devices
  - Scale-Up of Metal-Oxide Films and a-Si PV Devices
  - Energy and Cost Analysis

University of Hawaii
- Technical Management
  - Photoelectrode Integration
  - Sputtered Metal-Oxide Films
  - High-Efficiency PV Materials
  - Hydrogen Evolution Catalyst Development

Intematix Corp.
- Combinatorial Discovery of Novel Metal Oxide Films

SwRI
- Ion Beam Surface Modification
  - Large-Scale Metal-Oxide Fabrication

Duquesne University
- Spray-Pyrolytic Metal Oxide Films

NREL
- Device Performance Certification
  - 1st-Principle Calc. of Metal-Oxides
  - Alternative PEC Materials

UCSB
- Rapid PEC Screening Methods
Anticipated Progress *(no funding to date)*:  
1. Milestone Plan

<table>
<thead>
<tr>
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<th>Year 1</th>
<th>Year 2</th>
<th>Year 3</th>
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<tbody>
<tr>
<td><strong>HPE Demonstration:</strong></td>
<td>2-4% STH 200hr</td>
<td>5-7% STH 500hr</td>
<td>7.5% STH 1000hr</td>
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<td><em>Efficiency, lifetime targets</em></td>
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<td><strong>Materials R&amp;D:</strong> (PEC material)</td>
<td>1.7 -3.3 mA/cm², 200hr</td>
<td>4.1-5.7 mA/cm², 500hr</td>
<td>6.1 mA/cm², 1000hr</td>
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<tr>
<td><em>Photocurrent, Lifetime targets</em></td>
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<td><strong>Commercialization:</strong></td>
<td>Energy/Economics analysis report</td>
<td>Reel-to-reel cass. deposition of PEC materials/devices</td>
<td>Vacuum roll deposition of PEC materials</td>
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Anticipated Progress (no funding to date):  

2. Proposed Task Integration Chart
Anticipated Progress (no funding to date):  
3. Photoactive Materials R&D Target  
Performance of 6.1 mA/cm² with 1000hr durability - achieved through:

1. Combinatorial Discovery of PEC Materials (barrier AP):
   - Adaptation of combinatorial ion beam sputtering to metal oxide films
   - Development of high-throughput bandgap screening technique
   - Development of high-throughput PEC screening technique
   - Fabrication & screening of 1000s of metal oxide compounds

2. Advanced Analysis and High-Performance Materials (barrier AP,AQ):
   - Analysis of high-performance (high-temp. process) samples
   - PEC analysis (IPCE, Mott Schottky..)
   - Surface analysis (XRD, SEM, AFM)
   - Identification of suitable hosts and dopants by first-principles calculations

3. Film Modifications for efficiency and durability (barrier AP,AQ):
   - Ion beam texturing: effect on surface area, overpotentials/film stress
   - Ion implantation: controlled doping of PEC material

4. HPE-Compatible Process Development (barrier AP,AQ, AS):
   - Low-temperature sputter deposition of most promising compounds
Anticipated Progress *(no funding to date)*: 4. HPE Performance Target

Performance of 7.5% STH with 1000hr durability - achieved through:

1. Development of improved Hybrid Photoelectrodes (barrier AS):
   - Optimized HPE Design for best available PEC materials
   - HPE fabrication/device completion
   - Identification of failure modes/ durability issues

2. Production of customized photovoltaic devices for HPE (barrier AS):
   - Design of current-matched a-Si-based tandem devices
   - Fabrication of tandem devices with appropriate bottom- and top- layers
Anticipated Progress *(no funding to date)*: 5. Commercialization Targets

1. **Completion of Energy/Economic Analysis (barrier AT):**
   - Assessment of feasibility of large-scale implementation of HPE technology

2. **Demonstration of Intermediate Scale Fabrication of HPE Devices (barrier AR):**
   - Device fabrication using reel-to-reel cassettes* in a cluster tool environment

   *MVSystems patented approach for reel to reel cassette (US patent #6,258,408B1)

3. **Demonstration of Large Scale Fabrication of HPE Devices (barrier AR):**
   - Material fabrication using commercial-scale vacuum roll deposition system
Future Work

Necessary work for DOE 2010 goals:
• Material development to reach 8 mA/cm² (requires $E_G < 2.3$ eV for top-junction)
• Device optimization (bottom junctions) to reach 10% STH
• Plant design and construction, goal 8% STH, 1000 hrs min. lifetime

Necessary work for DOE 2015 goals:
• Material development to reach 10 mA/cm² (requires $E_G < 2.0$ eV for top-junction)
• Device optimization (bottom junctions) to reach 12% STH
• Plant design and construction, goal 10% STH, 5000 hrs min. lifetime
Publications and Presentations

None - no funding yet.
This project is new, and was not reviewed in 04.

The May 04 review included comments regarding PEC research in general:

“Sufficient funding in this area for long term development is lacking, however some progress was made since last year. A concern of reviewers is that this area represents a “splintered” collection of smaller projects, and that a dedicated, multi-disciplinary program that is well organized and integrated should be put in place”

*Response:* These comments are well founded and fairly accurate. The collaborative work initiated in this project represents a significant first step toward a well-organized and dedicated multi-disciplinary program to advance the development of commercial PEC hydrogen production systems.
Hydrogen Safety

The most significant hydrogen hazard associated with this project is:

Accumulation of small amounts of hydrogen during long-term testing of prototype devices.*

*at 7.5% STH efficiency under 1-sun, a 4 cm² lab-scale device produces less than 1 milligram of H₂ per hour.
Hydrogen Safety

Our approach to deal with this hazard is as follows:

• Utilize extensive hydrogen safety plans developed by HNEI for the “Hawaii Fuel Cell Test Facility”. Elements include:
  – Complete database of relevant codes and standards
  – Failure modes and effects analysis (FMEA)
  – Review by industrial partner of FMEA and safety compliance
  – Generation of in-house safety manuals

• For this project, MVSystems will implement the appropriate safety plans to accommodate the small quantities of hydrogen produced in the lab-scale PEC experiments*, including:
  – Specification of adequate ventilation of the laboratory space
  – Training of personnel in H₂ handling procedures & emergency protocols

*at 7.5% STH efficiency under 1-sun, a 4 cm² lab-scale device produces less than 1 milligram of H₂ per hour.