PROJECT facts

U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

Hydrogen and Clean Fuels from Coal

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High Permeability Ternary Palladium Alloy Membranes with Improved Sulfur and Halide Tolerance

CONTACTS

Richard Dunst
DOE Project Officer
National Energy Technology Laboratory
626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-6694
Fax: 412-386-5914
richard.dunst@netl.doe.gov

Daniel C. Cicero
DOE Technology Development Manager
National Energy Technology Laboratory
3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4826 or 412-386-6152
Fax: 304-285-4403
daniel.cicero@netl.doe.gov

Kenneth Coulter
Southwest Research Institute
6220 Culebra Road
San Antonio, TX 78238-5166
210-522-3196
kent.coulter@swri.org

Description

A critical step in the transition to the hydrogen economy is the separation of hydrogen from coal gasification gases (syngas) or methane. This is typically accomplished through membrane separation. Past research has shown that palladium (Pd) alloys possess great potential as robust and economical membranes. However, the search for the optimal binary or ternary alloys is an involved and costly process due to the immense number of alloy variations that could be prepared and tested. Recent modeling work at Georgia Institute of Technology using density functional theory (DFT) identified several promising ternary alloy compositions with improved hydrogen permeability. These promising ternary alloy compositions, along with various additives at different concentrations, are to be 'tested' via DFT calculations and used to guide experimental membrane development efforts.

Southwest Research Institute (SwRI) will lead this membrane advancement effort through the development of materials using advanced physical vapor deposition methods. These methods include high power pulsed magnetron sputtering and plasma enhanced magnetron sputter deposition to produce thin (<5 micron) Pd alloy membranes. The unique feature of these techniques is the ability to rapidly produce uniform membranes of almost any alloy composition with face surface areas up to 100 in^2.

The Colorado School of Mines (CSM) will perform initial screening of experimental membranes under controlled atmospheres to confirm that the targeted structures and compositions have been produced. Test results will be used to guide and refine DFT-based modeling and guide the vacuum deposition effort. When one or more promising classes of ternary alloys have been identified, TDA Research will evaluate these membranes under different concentrations of hydrogen sulfide (H_2S), hydrogen chloride (HCl), nitrogen (N_2), and other contaminants for extended periods up to several hours. Synergistic effects, if any, are also to be examined.

Primary Project Goals

- Using DFT modeling, develop an expanded range of ternary alloy compositions and additive concentrations to guide materials development efforts.
- Produce thin (<5 micron) Pd alloy membranes using advanced physical vapor deposition methods, including high power pulsed magnetron sputtering and plasma enhanced magnetron sputter deposition.

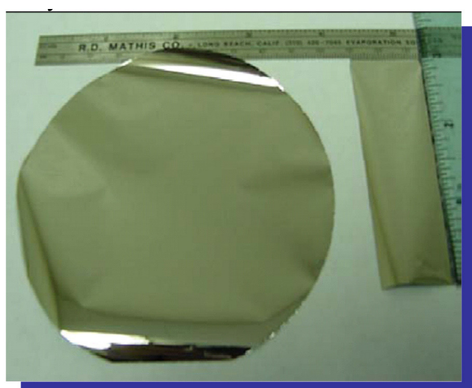
- Perform initial screening of experimental membranes under controlled atmospheres. Confirm targeted structures and compositions have been produced.
- Evaluate promising classes of ternary alloys as membranes under different concentrations of H_2S, HCl, N_2, and other contaminants.

Accomplishments

- Tested seven ternary alloys for hydrogen permeation rates under pure gas experiments. Tests were conducted under a range of pressures (5 to 150 pounds per square inch gauge [psig]) and temperatures (200 to 500 °C).
- Demonstrated that the addition of four weight percent silver (Ag) to a palladium-copper (Pd-Cu) alloy membrane improves the permeability by 20 to 25 percent.
- Used computer modeling to predict unique alloy compositions that showed (theoretic) excellent hydrogen solubility and permeability. These compositions are being validated through laboratory tests.
- Evaluated promising classes of ternary alloys as membranes under different concentrations of H_2S, HCl, N_2, and other contaminants.

Benefits

Self-supporting, dense Pd alloy membranes have exhibited extremely high hydrogen permselectivity and the ability to produce high purity hydrogen feed streams needed for fuel cell applications. The combinations of binary and ternary alloys that can be produced with Pd are theoretically infinite. The use of DFT modeling is an economical and efficient approach to identify promising alloy combinations, which can then be fabricated and evaluated to determine optimum alloy combinations.



SWRI Membrane

ADDRESS

National Energy Technology Laboratory

1450 Queen Avenue SW
Albany, OR 97321-2198
541-967-5892

2175 University Avenue South
Suite 201
Fairbanks, AK 99709
907-452-2559

3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4764

626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4687

One West Third Street,
Suite 1400
Tulsa, OK 74103-3519
918-699-2000

CUSTOMER SERVICE

1-800-553-7681

WEBSITE

www.netl.doe.gov