PROJECT facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

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HIGH PERMEABILITY TERNARY PALLADIUM ALLOY MEMBRANES WITH IMPROVED SULFUR AND HALIDE TOLERANCE

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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 by a membrane. Past research has shown that palladium (Pd) alloys show great promise as robust and economical membranes. However, the search for the optimal binary or ternary alloy is an involved and costly process due to the infinite number of alloy variations that could be prepared and tested. Recent modeling work at the Carnegie Mellon University 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 may be tested via DFT calculations and used to guide experimental materials development efforts in an iterative manner.

Southwest Research Institute (SwRI) will lead the materials development effort using advanced physical vapor deposition methods including 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 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. Once one or more promising classes of ternary alloys have been identified, TDA Research will evaluate these membranes under different concentrations of H_2S, HCl, N_2, and other contaminants for extended periods, up to several hours. Synergistic effects, if any, may also be examined.

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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

None at present – New project initiated in FY-2007.

Benefits

Self-supporting, dense palladium alloy membranes have been shown to exhibit extremely high hydrogen permselectivity and are able to produce high purity hydrogen feed streams needed for fuel cell applications. The combinations of binary and ternary alloys that can be produced with palladium are theoretically infinite. Consequently, the cost involved with constructing and testing each alloy combination will also be large. The use of DFT modeling is an economical and quick approach to identify promising alloy combinations that can be then fabricated and evaluated to determine optimum alloy combinations.