IV.D.3 Development, Selection and Testing to Reduce Cost and Weight of Materials for BOP Components

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Subcontractor:
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Project End Date: March 31, 2018

Overall Objectives

- Reduce weight of structural stainless steels for balance of plant (BOP) components by 50%.
- Reduce cost of structural stainless steels for BOP components by 35%.
- Expand the technical basis for selecting a diverse set of austenitic stainless steels for materials of construction in BOP components.
- Identify simplified testing procedures to enable materials qualification.

Fiscal Year (FY) 2017 Objectives

- Assess fatigue strength, material weight and cost of several engineering alloys in a representative hydrogen environment, including a technologically relevant gall resistance austenitic stainless steel and a low-Ni, high-strength austenitic stainless steel.
- Evaluate consistency of reduced-order model of stacking fault energy with first-principles calculations.
- Develop publicly accessible framework for visualization of computation output (both reduced order models and results from first principles calculations) and other relevant metrics such as cost and nickel equivalent.
- Document the technical basis for selection of materials that satisfy the targets of this program in the context of fatigue performance, as well as a user manual for the web-based design tool.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section of the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan:

(A) System Weight and Volume

(B) System Cost

(H) Balance-of-Plant (BOP) Components

Technical Targets

No specific technical targets have been set. This project is a basic study of materials of construction for BOP with the goals of identifying lower-cost alternatives to the baseline of annealed Type 316L that can be implemented in lighter-weight designs. The project targets are:

- Reduce weight of structural stainless steels for BOP components by 50%.
- Reduce cost of structural stainless steels for BOP components by 35%.

FY 2017 Accomplishments

- Several low-nickel alloys have been shown to have similar fatigue performance in gaseous hydrogen as the benchmark material, Type 316/316L austenitic stainless steel, for relevant allowable design stresses.
- Several high-strength alloys have been shown to display similar fatigue performance in gaseous hydrogen as the benchmark material, Type 316/316L austenitic stainless steel, but at higher applied stress.
- Estimated component weight and cost savings from alloys with the combination of low nickel composition and high strength can be greater than 50% and 40% respectively, and could be as high as 70% and 60% in some cases.
- A web-based, user-friendly (and expandable) design tool has been developed for visualization and multi-variable optimization of compositionally-derived materials characteristics, such stacking fault energy, martensite transformation temperature, nickel equivalent and cost. The tool allows calculation of materials characteristics from reduced order models, or interpolation from databases of first principles calculation results.
- More than 4,000 alloy compositions have been screened for stacking fault energy and incorporated into the alloy design tool.

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INTRODUCTION

The primary objective of this effort is to identify alloys to replace Type 316/316L in hydrogen service for BOP applications onboard fuel cell electric vehicles. Type 316/316L austenitic stainless steels are used extensively in hydrogen systems for their resistance to hydrogen embrittlement, which is attributed to the relatively high nickel content of Type 316/316L alloys. Nickel content, however, drives the cost of austenitic stainless steels, thus Type 316/316L alloys impose a cost premium compared to similar alloys with lower nickel content. Since the cost of BOP components is a large fraction of the cost of hydrogen fuel systems (even dominating the cost at low production volumes [1]), alternative materials are desired. In addition, Type 316/316L alloys are relatively low strength, thus high-pressure components tend to be heavy to accommodate the stresses associated with the pressure loads. Higher-strength materials enable reduction of weight of BOP components and contribute to lower cost since less material is needed. However, engineering data to justify selection of lower cost and higher strength alloys for high-pressure hydrogen service are currently unavailable.

Additionally, high-throughput computational materials science has evolved to a level of sophistication that large databases of composition can be screened based on knowledge of sensitive performance metrics. While first-principles prediction of fatigue performance is still beyond the capability of computational materials science, many intrinsic behaviors of alloys can be predicted from first principles. This effort uses stacking fault energy, which can be calculated, as an indicator of resistance to hydrogen embrittlement to screen large compositional space. Databases of these calculations are combined into an interactive tool where a user can assess multiple compositionally-sensitive attributes to design new alloy compositions. In this case, alloy compositions that optimize cost and hydrogen resistance (through the stacking fault energy indicator).

APPROACH

The objective of this project is addressed from two perspectives: (1) experimental evaluation of commercial alloys and (2) computational materials discovery of new alloys. In the first case, fatigue properties in hydrogen environments are evaluated for low-cost, high-strength alloys and compared to the benchmark of annealed Type 316/316L. The test program seeks appropriate trade-offs between materials cost and performance, such that hydrogen embrittlement can be effectively managed in design for BOP components onboard fuel cell vehicles where the anticipated number of refuelings is significantly less than 10^4 pressure (fatigue) cycles. Performance includes fatigue at low temperature associated with refueling protocols at -40°C; the effect of hydrogen on fatigue as a function of temperature has not been previously reported. An additional goal of the experimental activity is to demonstrate a straightforward, simplified methodology by which materials may be qualified for safe hydrogen service, including the use of internal hydrogen (saturation of the material with hydrogen by thermal precharging) as a robust substitute for testing in gaseous hydrogen.

The goal of the computational discovery activity, like the experimental activity, is to identify low-Ni content (and thus lower cost) stainless steel alloys for use in BOP components. To achieve this goal from a computational perspective, a framework has been developed to screen compositionally-derived characteristics of austenitic stainless steels in relevant trade spaces. Screening can be performed based on optimization of cost and performance metrics and can be expanded to include additional materials characteristics. The evaluation framework uses databases of performance metrics based on stacking fault energy (an indicator of resistance to hydrogen) derived by either a reduced-order thermodynamic model or ab initio calculations. This effort represents a new initiative in the DOE Fuel Cell Technologies Office research portfolio to use computational materials science coupled with high-performance computing to aid materials development. This innovative approach will provide the DOE and U.S. industry with a framework and computational tools to efficiently and effectively explore the design space for next-generation materials used in fuel cell technologies.

RESULTS

Materials Selection and Fatigue Characterization

The fatigue behavior of a diverse range of austenitic stainless steels have been characterized in several hydrogen environments. The tested alloys include high-strength conditions of common 304L and 316L austenitic stainless steels; a high-strength, low-nickel austenitic stainless steel used for heat exchanger tubes (XM-11); a gall-resistant austenitic stainless steel in a high-strength condition (Nitronic 60); and a nitrogen-strengthened, low-nickel austenitic stainless steel for resistance to rotating fatigue (SCF-260). Table 1 provides the strength and major alloying elements for the tested alloys.

Weight and cost savings of the tested alloys were estimated by considering a cylindrical shell using the minimum required wall thickness according to the ASME code for Hydrogen Piping and Pipelines (ASME B31.12). The maximum allowable stress in the wall thickness calculation is 1/3 of the minimum specified tensile strength (or 2/3 of the yield strength, whichever is lower) from relevant materials specifications. The weight reduction of a given alloy represents the difference between the alloy and the annealed 316L benchmark. The cost reduction is realized by using less material (proportional to weight) and by assuming the material cost per kilogram is proportional to the sum of the nickel content and half of the manganese content. As shown in Table 1, the upper bound weight and cost savings are projected to be greater than 50%.

The projected cost and weight savings are substantial, but the simple analysis assumes that the fatigue limit in hydrogen is greater than the allowable stress; in other words, the design stress is limited by the characteristic strength of the alloy and not by the fatigue performance. Prior to this study, there was no available fatigue life data for high-strength austenitic stainless steels in gaseous hydrogen. Additionally, the effects of hydrogen on fatigue at low temperature was largely unknown. In general, the fatigue life of austenitic stainless steels at room temperature is relatively insensitive to pressure (Figure 1). Moreover, the fatigue life in gaseous hydrogen at pressure of 10 MPa at low temperature was found to be greater than the fatigue life at room temperature (for the same applied stress; Figure 2). Nitronic 60 is the only exception to these trends, but still displays a fatigue life similar to the other alloys for allowable stresses greater than 300 MPa. While the combination of high-pressure hydrogen and low temperature remains to be tested, these data suggest that fatigue testing at low temperature may not be necessary to qualify austenitic stainless steels for vehicle applications (if pressure insensitivity is maintained at low temperature). It is important to recognize that all of the data in Figures 1 and 2 represents notched specimens and are conservative relative to conventional smooth test specimens; however, in all cases, fatigue life of more than 10^5 cycles can be achieved for allowable stresses less than 200 MPa, demonstrating infinite life in the vehicle context that is superior to the benchmark of an allowable stress of 115 MPa (i.e., superior to annealed 316L).

Computational Materials Discovery

While stacking fault energy has been shown to be a first-order screening metric for assessing hydrogen effects on tensile ductility, stacking fault energy is not predictive of tensile properties and does not correlate with fatigue behavior. Stacking fault energy, however, remains an important characteristic of the deformation character of austenitic alloys. The stacking fault energy of more than 4,000 alloy compositions, consisting of Fe, Ni, Cr, Mn, Mo and Si, have been calculated using the coherent potential approximation with density functional theory. The data revealed several alloys with low Ni content and relatively large stacking fault energy. We are currently in the process of expanding the data set to include alloys containing Al and Cu. The general utility of high-throughput calculations, however, is limited without methods to analyze and visualize these data.

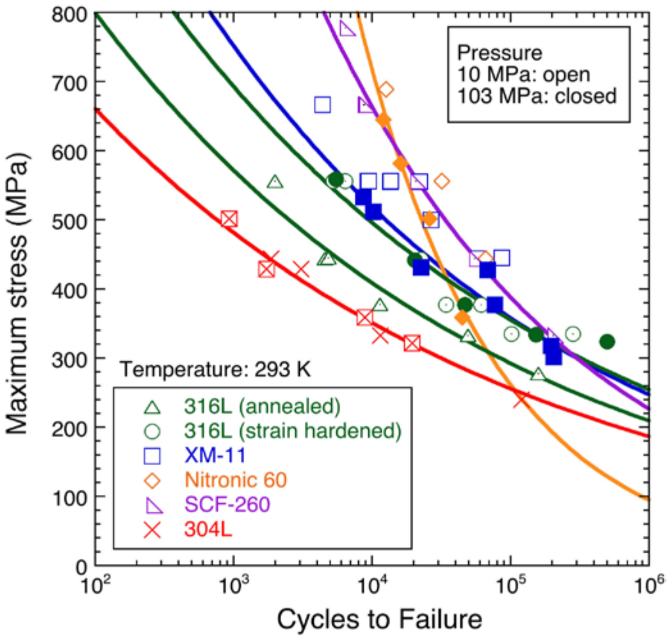


FIGURE 1. Fatigue life curves of notched specimens (K_t ~ 3.9) at room temperature for hydrogen pressure of 10 MPa and 103 MPa show little effect of pressure. Load ratio and frequency are 0.1 and 1 Hz, respectively.

To address this limitation, a user-friendly, web-based, materials-screening tool has been developed with the goal of providing an expandable and flexible platform to visualize large data sets and explore empirical metrics (or reduced order models) over large parameter spaces.

TABLE 1. Characteristics of Tested Austenitic Stainless Steels as Well as Projected Weight and Cost Savings (CW = Strain-Hardened to High Strength).

Alloy	Cr (wt%)	Ni (wt%)	Mn (wt%)	N (wt%)	Sy (MPa)	Su (MPa)	Allowable stress (MPa)	Weight savings (%)	Cost savings (%)
316L	17.5	12	1.2	0.04	280	562	115	–	–
CW 316L	17.5	12	1.2	0.04	573	731	218	72	58
CW 304L	18.3	8.2	1.8	0.056	497	721	195	66	65
XM-11	20.4	6.2	9.6	0.26	539	881	207	69	59
Nitronic 60	16.6	8.3	8.0	0.16	880	1,018	218	72	60
SCF-260	19.1	3.3	17.4	0.64	1,083	1,175	333	85	77

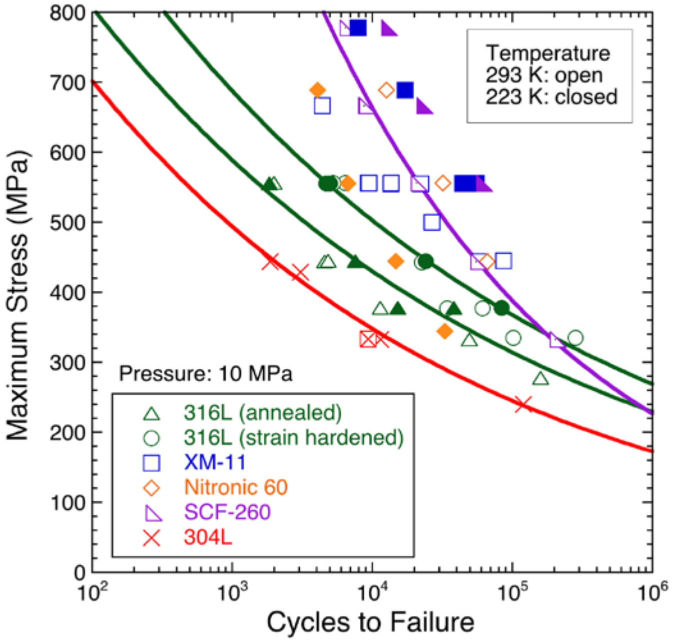
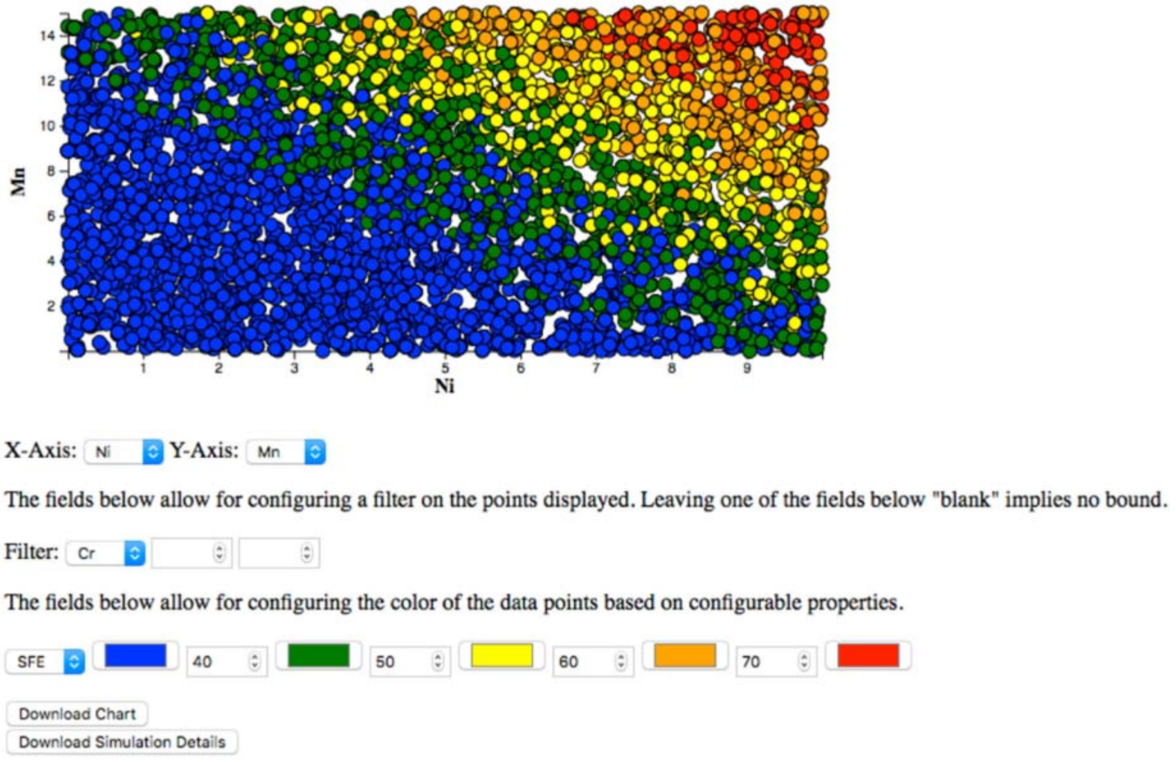


FIGURE 2. Fatigue life curves of notched specimens (K_t ~ 3.9) at hydrogen pressure of 10 MPa and temperature of 223 K and 293 K generally show room temperature represents limiting fatigue performance; Nitronic 60 appears to be a notable exception. Load ratio and frequency are 0.1 and 1 Hz, respectively.

Example output from the tool is shown in Figure 3: a color-contour plot of stacking fault energy in nickel manganese compositional space. In this case, the stacking fault energy is calculated with a reduced-order thermodynamic model. Each of the parameters can be filtered to further screen the parameter space displayed; for example, the plotted data can be restricted to a user-defined compositional range of chromium and/or other elements. The tool is also capable of visualizing other databases of information in the same manner, such as the density functional theory/coherent potential approximation output or any tabular data that exists in a comma-separated values file. In addition to empirical relationships for martensite transformation temperature and nickel equivalent, the tool currently includes also a framework for estimating cost based on the elemental composition. Visualization in this manner enables alloy optimization for parameters of interest as well as parametric studies of variance due to the allowable variation in composition; austenitic stainless steels have large specified compositional ranges (e.g., nickel content in type 316L can vary between 10 wt% and 14 wt% in most public materials specifications).



X-Axis: Ni Y-Axis: Mn

The fields below allow for configuring a filter on the points displayed. Leaving one of the fields below "blank" implies no bound.

Filter: Cr

The fields below allow for configuring the color of the data points based on configurable properties.

SFE 🟦 40 🟩 50 🟨 60 🟧 70 🟥

FIGURE 3. Screen-shot of the web-based, materials-screening tool shows color contours representing stacking fault energy plotted in nickel-manganese compositional space.

CONCLUSIONS AND UPCOMING ACTIVITIES

- A diverse range of austenitic stainless steels show acceptable fatigue performance for allowable stresses greater than the benchmark of annealed 316L; in other words, the fatigue life is greater than 10^5 cycles for maximum fatigue stress of 1/3 of the tensile strength (for load ratio of 0.1 and frequency of 1 Hz).
- Potential significant weight savings of more than 60% can theoretically be achieved for a range of alternatives to annealed 316L in BOP components. These weight savings translate to cost savings of more than 50% and potentially in excess of 60% for optimized designs.
- A user-friendly analysis tool has been developed to compare materials metrics based on composition. A database of stacking fault energy from more than 4,000 alloy density functional theory calculations can be probed, or the reduced-order thermodynamic calculation of stacking fault energy can be used as a comparison metric. Other comparison metrics (such as cost, nickel equivalent and martensite transformation temperature) can also be evaluated and other metrics can be added to the flexible alloy comparison tool.
- Testing capability for the combination of high pressure and low temperature is needed to confirm the hypotheses that (i) the limiting fatigue behavior can be established at room temperature (rather than at low temperature) and (ii) limiting behavior can be potentially established at pressure lower than the design pressure.
- Further weight and cost reductions can be achieved in less-conservative, finite-life designs (i.e., designing for higher fatigue stresses). To enable finite-life designs, the foundational mechanisms of hydrogen-assisted fatigue must be better understood and a design framework must be established to quantitatively capture the mechanical behavior of short cracks in hydrogen environments.

FY 2017 PUBLICATIONS/PRESENTATIONS

1. K.A. Nibur, P.J. Gibbs, J.W. Foulk, C. San Marchi: "Notched fatigue of austenitic alloys in gaseous hydrogen," (PVP2017-65978), Proceedings of the 2017 ASME Pressure Vessels & Piping Conference, 16–20 July 2017, Waikoloa, HI.

2. P.J. Gibbs (presenter), P.D. Hough, K. Thuermer, B.P. Somerday, C. San March, J.A. Zimmerman: "Stacking fault energy based alloy identification for hydrogen compatibility," presented at TMS 2017, 26 February–2 March 2017, San Diego, CA.

3. P.J. Gibbs, K.A. Nibur, C. San Marchi: "Plastic ratcheting and fatigue crack formation in austenitic steels with hydrogen," 2016 International Hydrogen Conference, 11–14 September 2016, Moran, WY, paper accepted for publication in proceedings, ASME 2017.