Innovative Development, Selection and Testing to Reduce Cost and Weight of Materials for BOP Components

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DOE Hydrogen and Fuel Cells Program Annual Merit Review

June 9, 2016

Project ID# ST113

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U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration
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Overview

Timeline

- Project start date: July 2014
- Project end date: Sept 2017

Technical Barriers

A. System Weight and Volume
B. System Cost
H. Balance-of-Plant (BOP) Components

Budget

- Total Project Budget: $2.4M (3 yrs)
  - Total Federal Share: $2.1M
  - Total Partner Share: $0.3M
  - Total DOE Funds Spent: $0.2M

Partners

- *Hy-Performance Materials Testing*
  - Subcontractor: fatigue evaluation in hydrogen
- *Swagelok Company*
  - In-kind: materials, test specimens, design perspective
- *Carpenter Technology*
  - In-kind: materials manufacturing expertise

Relevance and Objectives

Objective: Identify alternative to high-cost metals for high-pressure BOP components

Barrier from 2012 Storage MYRDD	Project Goal
A. System Weight and Volume	Reduce system weight by 50% Weight can be reduced by optimization of structural stresses
B. System Cost	Reduce system cost by 35% Cost can be reduced by selecting lower cost materials and using less material
H. Balance-of-Plant (BOP) Components	Expand the scope of materials of construction for BOP Appropriate materials should be determined by relevant performance metrics such as fatigue properties

Project Approach

<u>*Objective*</u>: Identify low-cost, lighter-weight alternatives to type 316L austenitic stainless steels

- *Reduced nickel* content is prime candidate for *cost reduction*
- *High-strength* is prime candidate for *weight reduction*

1. Evaluate fatigue properties of austenitic stainless steels in hydrogen environments
   - Benchmark existing "standard": annealed type 316L
   - Evaluate alloys with lower-nickel content
   - Evaluate alloys in higher-strength condition
2. Computational materials discovery
   - Correlate stacking fault energy (SFE) with hydrogen effects
   - Develop high-throughput computational strategy to determine SFE
   - Use computational strategy to explore alloy additions to increase SFE
3. Fabricate and evaluate new alloy combinations (based on computations)
   - Fatigue performance in hydrogen environments (experimental)

Simple analysis suggests significant cost and weight reductions can be realized

- Relative component cost is estimated from the relative weight of material and material cost
  - Relative weight is determined from required thickness of material
  - Relative material cost is conservatively informed from price of bar material

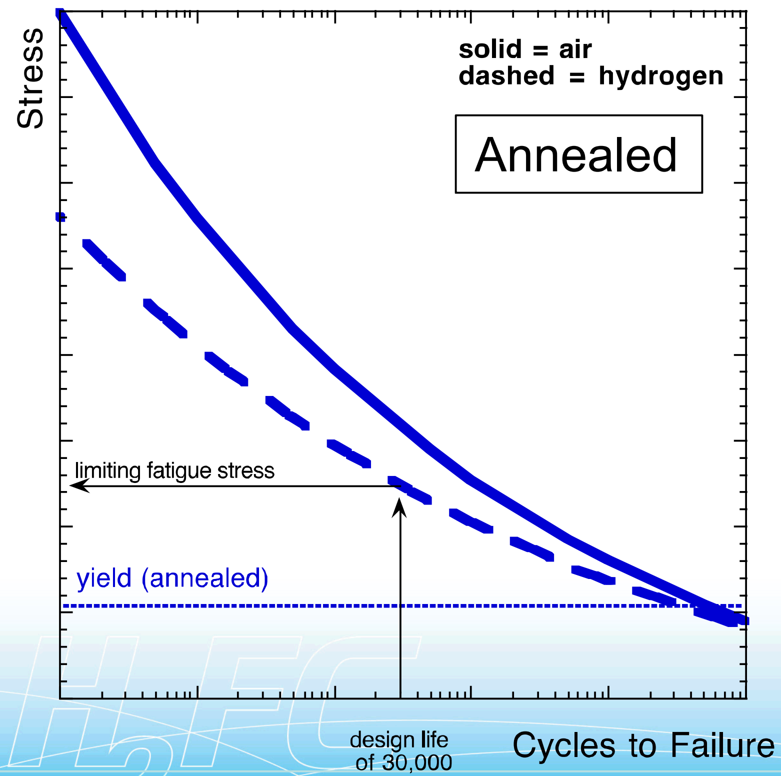
$$t = \frac{PD}{2(SE + PY)}$$ ASME design equation

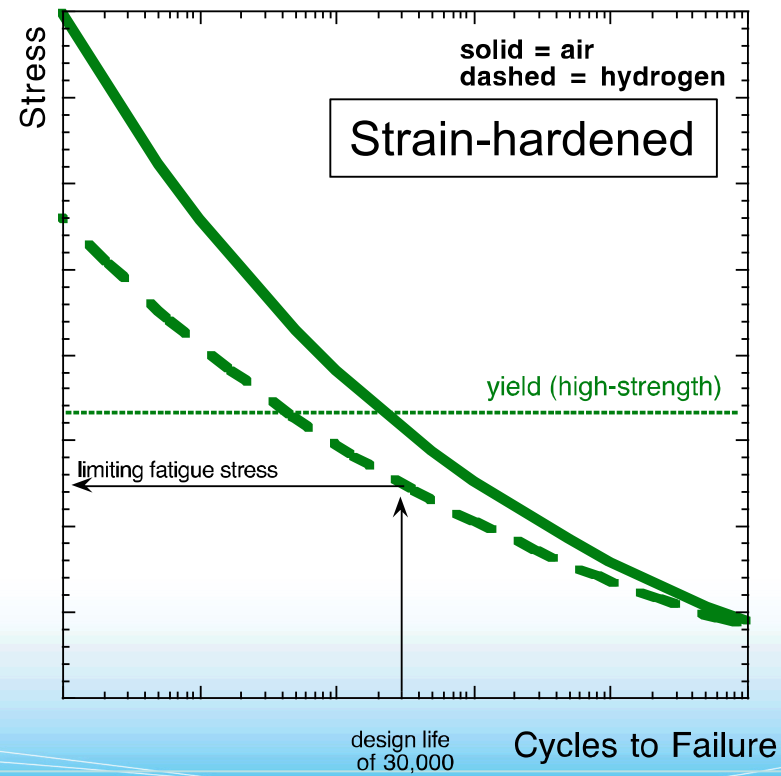
material	Relative material cost	Yield strength (MPa)	Relative weight	Relative component cost
316L	1.0	140	1.0	1.0
304L	0.84	140	1.0	0.84
CW 304L	1.7	345	0.46	0.78
XM-11	0.79	345	0.46	0.36
CW XM-11	1.6	620	0.17	0.27
CW XM-19	2.5	725	0.15	0.38

Project Approach

Use stress-based fatigue method for hydrogen from the public domain (CSA CHMC1)

- By increasing the strength, higher fatigue stresses can be accommodated in design
  - Higher stress = less material
  - Less material = lower cost



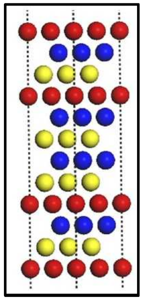


Project Approach

Density functional theory (DFT) enables prediction of fundamental characteristics that correlate with hydrogen effects

- Implement software needed to interface VASP and Dakota to estimate SFE
- Quantify uncertainties in these calculations
- Intelligently explore compositional 'space'

quantum calculations to estimate SFE for a given alloy



database to store calculation results and feedback to Dakota algorithms

Fe	Cr	Ni	Mn	Al	SFE	δ_{SFE}	Notes
74	18	8	---	---	15	5.0	304L
68	12	8	10	2	32	6.2	10-8-2.5
70	17	13	---	---	40	2.0	316L
50	15	8	22	5	---	---	unstable
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algorithms guiding alloy composition selection to maximize SFE and minimize Ni content

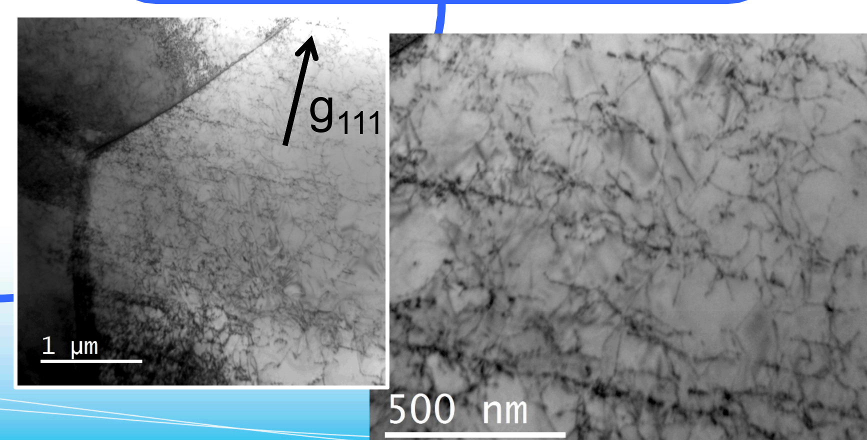
Project Approach

Use SFE database to develop computationally inexpensive surrogate models and a model design tool

design and fitting of surrogate model forms and parameters to database

analysis and validation of SFE-composition relation

$$SFE = f(\%Cr, \%Ni, \%Mn, \%Al) \pm g(\%Cr, \%Ni, \%Mn, \%Al)$$

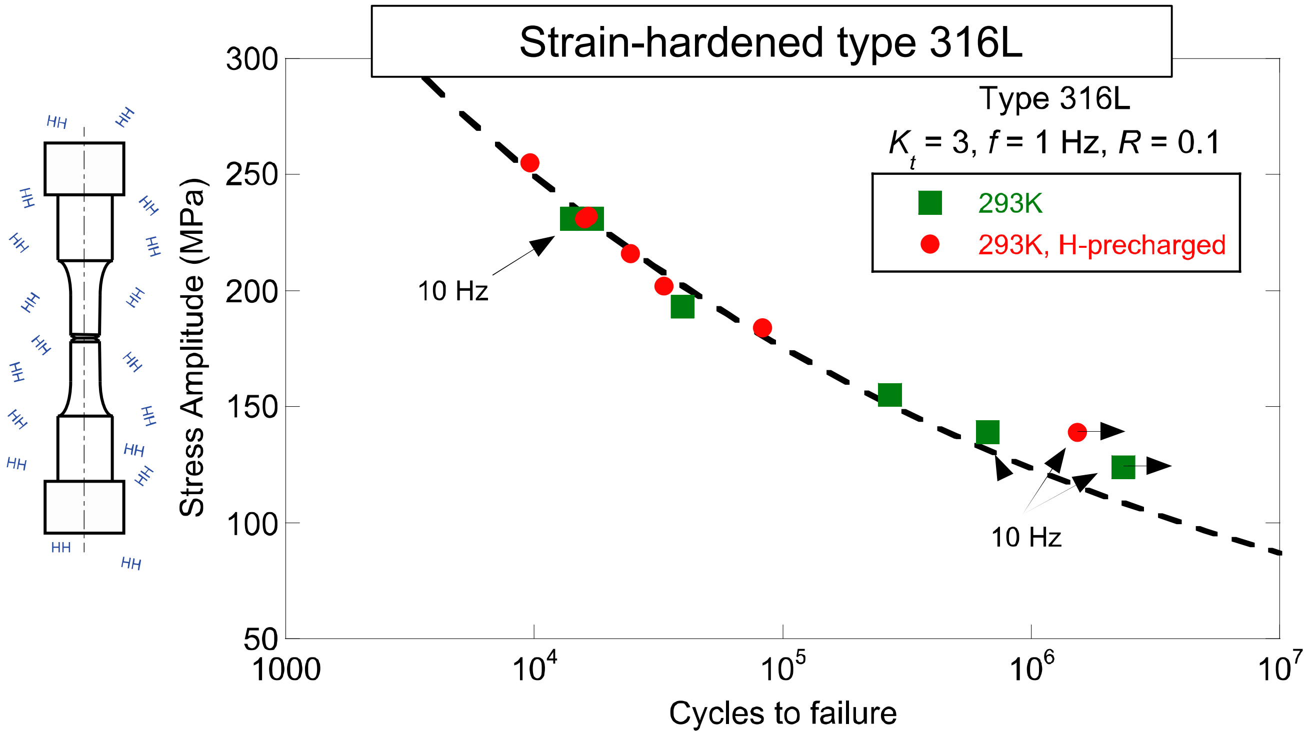


Project Approach and Milestones

Milestone	Target date	Status
Fatigue life measurements at low temperature (baseline material)	FY15Q2	High-strength alloy selected for initial testing (70% complete)
Fatigue life measurements in gaseous hydrogen (baseline material)	FY15Q3	Testing started at HPMT (25% complete)
VASP calculations for Ni and for Fe-Cr-Ni	FY15Q2	Predictions for Ni are consistent with literature (50% complete)
Go-No Go Establish correlations between SFE and experimentally measured metrics	FY15Q4	Data from literature is incomplete
Go/No Go Provide basis for meeting cost and weight targets with commercial alloys	FY16	XM-11 selected; initial tests started (5% complete)
Go/No Go Identify one or more candidate materials that potentially meet project goals	FY16	No significant results

Accomplishment:

Baseline fatigue performance established for high-strength type 316L



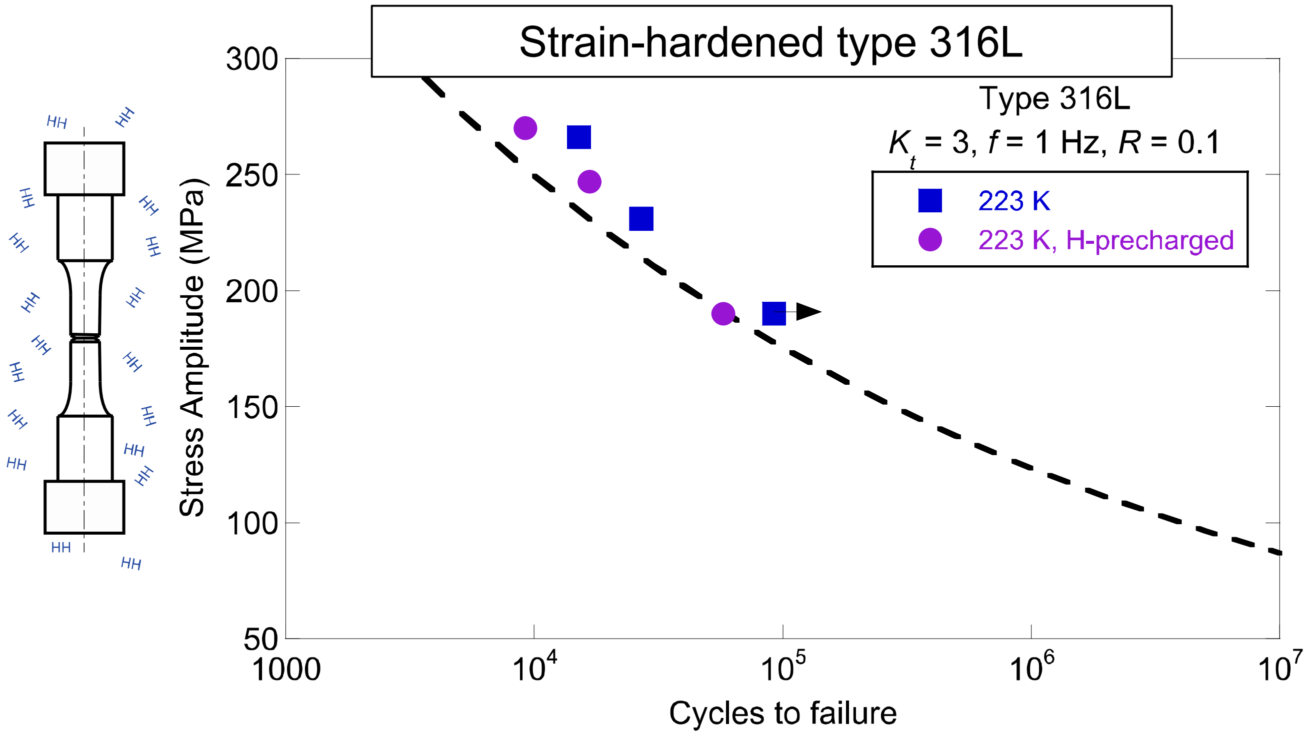
Notched tension-tension fatigue

- Ni = 12.04 wt%
- Sy = 589 MPa
  - S_A = 265 MPa (R = 0.1)
- Su = 967 MPa

- High fatigue stress can be achieved with cycles to failure greater than 10,000 cycles (200 years of weekly filling)
- Broader evaluation of performance requires testing at low temperature

Accomplishment:

Low-temperature results show non-limiting performance

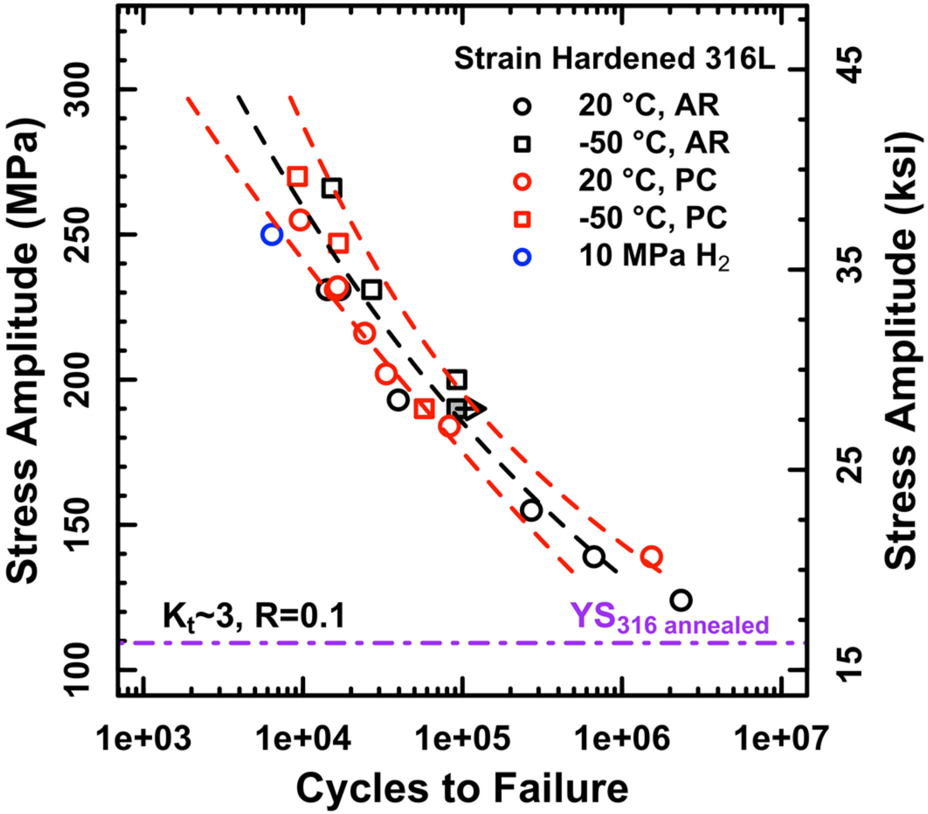


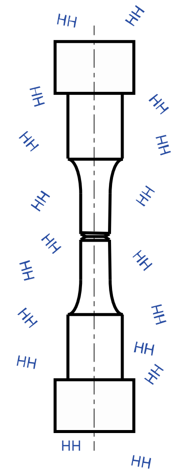
Notched tension-tension fatigue

- Ni = 12.04 wt%
- Sy = 589 MPa
  - S_A = 265 MPa (R = 0.1)
- Su = 967 MPa

- Low-temperature fatigue life is “as good as or better” than fatigue life at room temperature
- Broader evaluation of methodology requires testing in gaseous hydrogen at low temperature

Accomplishment:
Fatigue life testing in gaseous hydrogen has begun





Notched tension-tension fatigue

- Ni = 12.04 wt%
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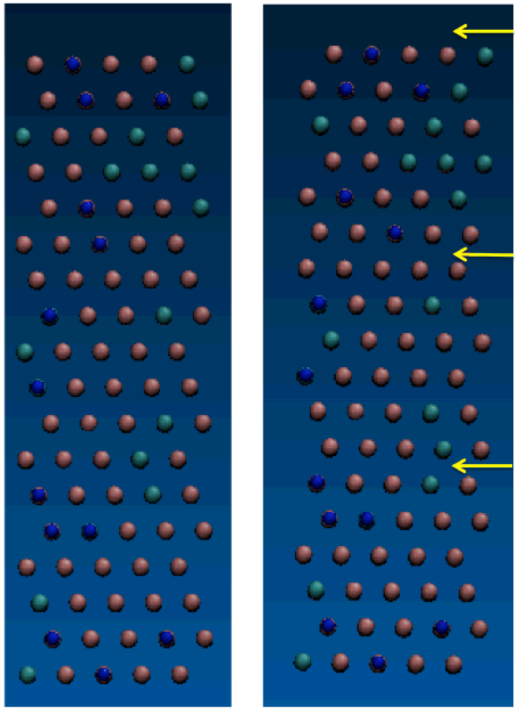
- Hy-Performance Materials Testing (HPMT) is performing fatigue tests in gaseous hydrogen at pressure of 10 MPa
- HPMT has demonstrated low-temperature tests in gaseous hydrogen for other configurations

Accomplishment:

Ab Initio Calculation of Stacking Fault Energy

- Quantified SFE for fcc Ni using supercell geometries
  - Value is consistent with known literature
  - Value is not sensitive to local magnetic moment
- Assessed computational effort for ternary (Fe-Cr-Ni) stainless steel alloy
  - 450 atoms per supercell needed to ensure system symmetries and small variations in total energies
  - SFE values are sensitive to magnetic moment, resulting in long energy relaxation times

DFT simulation



ternary alloy bulk crystal | ***crystal with inserted stacking faults***

Collaborations and Partnerships

- Sandia National Laboratories
  - Core DOE capability for high-pressure hydrogen testing
  - Leverage between NNSA and EERE customers
  - Deep expertise in mechanical metallurgy of austenitic stainless steels
  - Advanced computing tools
- Hy-Performance Materials Testing (Kevin Nibur)
  - Commercial testing expertise in pressure environments
  - Unique capabilities in the US
- Swagelok Company (Shelly Tang)
  - Component manufacturer
  - Materials selection and engineering analysis
  - Deep understanding of manufacturing with austenitic stainless steels
- Carpenter Technology (Sam Kernion)
  - Steel manufacturer
  - Metallurgical expertise and cost analysis

Remaining Challenges and Barriers

- **Challenge**: Fatigue testing at low frequency requires long time (3 days ~ 250K cycles at 1 Hz).
- **Resolution**: Focus on high stresses, i.e., cycles to failure of 10,000-30,000 cycles

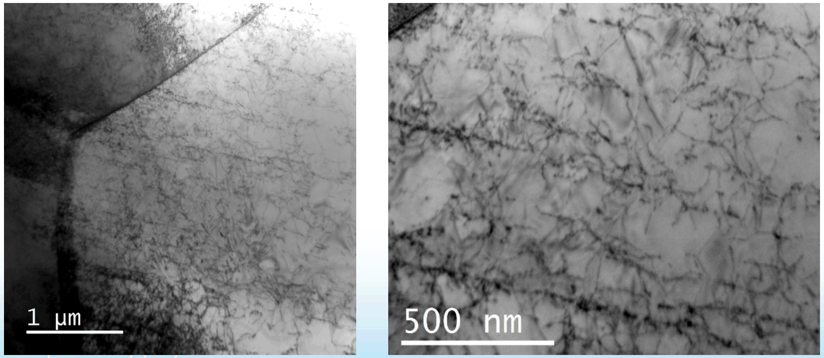
- **Challenge**: Unclear whether existing literature will provide clarity on correlations between SFE, mechanical properties and HE-resistance.
- **Resolution**: Focus effort on establishing correspondence between relative value and ordering of SFE for various alloy compositions, and known mechanical behavior from experimental side of project and engineering literature.

- **Challenge**: Currently examining extent to which temperature-related contributions to free energy affect SFE values. If influence is significant, high throughput nature of calculations may be compromised.
- **Resolution**: Use simple compositions to establish the magnitude of this effect, and its computational cost/speed relative to the overall calculations.

Proposed Future Work

Remainder of FY15:

- Complete testing of 316L (benchmark) and commence testing of XM-11 (low-nickel alloy)
- ***Go/No Go***: Demonstrate fatigue life test method (CSA CHMC1) for all environments
- Perform transmission electron microscopy (TEM) and analysis to quantify SFE values for select stainless steel alloys; validate SFE calculations.
  - 316L
  - Fe-Cr-Ni-Mn-Al austenitic stainless steel alloys: IJHE 38 (2013) 9935-9941
  - XM-11 (Fe-21Cr-6Ni-9Mn austenitic stainless steel)



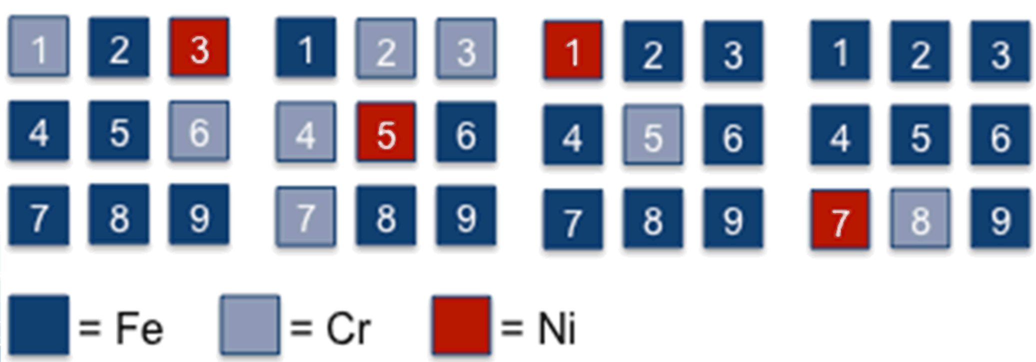
TEM images showing dislocation microstructure in Fe-13Cr-8Ni-10Mn-2.5Al alloy

alloy provided by Naumann (BMW) and Michler (Adam Opel/GM)

Proposed Future Work

Remainder of FY15:

- ***Go/No Go***: Demonstrate correlation between SFE values, mechanical properties and hydrogen embrittlement resistance
- Computationally quantify SFE for commercial alloys and Fe-Cr-Ni-Mn-Al alloys
  - 316L, XM-11, Fe-13Cr-8Ni-10Mn-2.5Al
  - Include temperature effects through magnetic entropy contribution to energies
- Develop space-filling sampling strategy to explore effects of different configurations with the same composition on stacking fault energy
- Explore permutation techniques to make baseline samples consistent with target composition

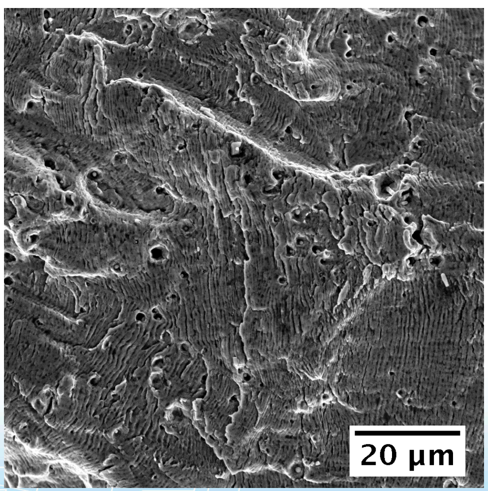


Use Monte Carlo approach to generate a sample of configurations that ensures confidence that the sample size is sufficient.

Proposed Future Work

FY16:

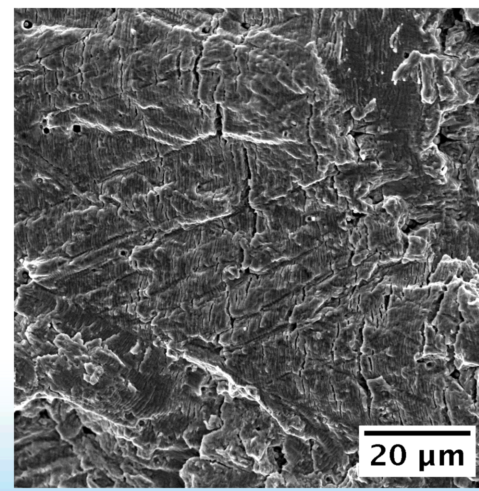
- Establish quantitative comparison of fatigue performance between benchmark and low-nickel alloys
- ***Go/No Go***: Provide basis for meeting cost and weight targets through materials selection of commercial alloys
- Explore extrapolation of data to
  - design (e.g., collaboration with Swagelok)
  - other fatigue methodologies (e.g., non-notched geometry and crack growth)



Fatigue fracture surfaces
Test temperature = -50 °C

As-received
S_A = 200 MPa

H-precharged
S_A = 190 MPa



0.7 µm/cycle

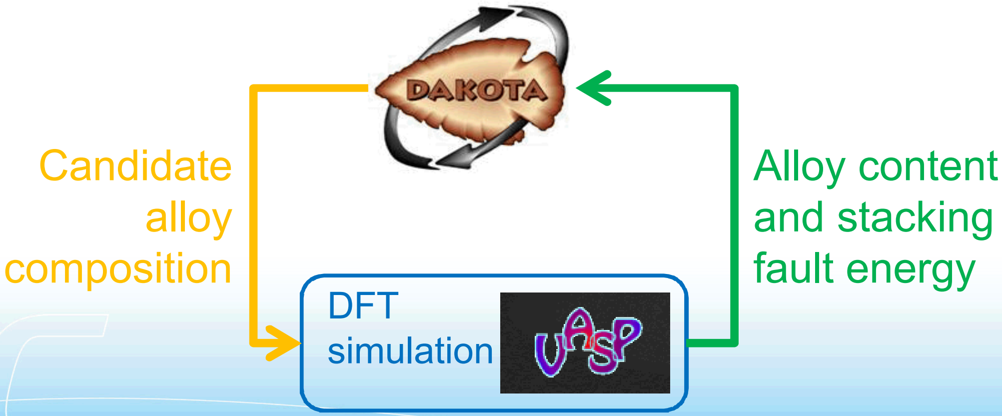
Crack Growth Direction →

0.6 µm/cycle

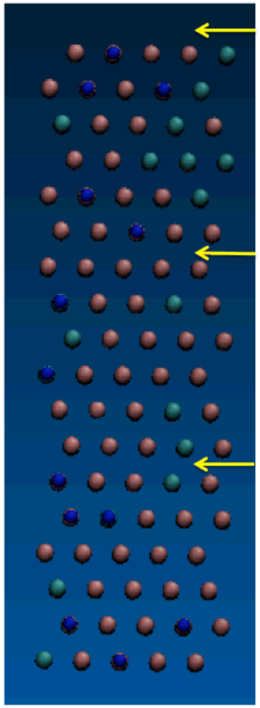
Proposed Future Work

FY16:

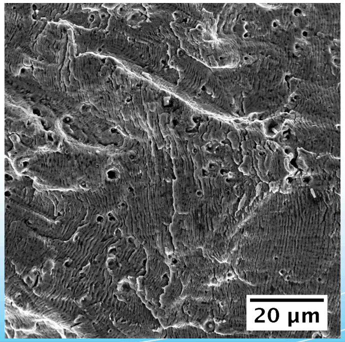
- Create software infrastructure to optimize alloy composition and robustness tradeoffs. Perform prototype studies to compare candidate approaches
- Perform preliminary set of optimized calculations and assemble initial version of SFE database. Deliver set to Carpenter Technology Corporation for feedback
- Perform analysis of calculated compositions to quantify trends in estimated SFE and uncertainty. Use Carpenter feedback to extend database
- ***Go/No Go***: Identify one or more candidate materials that potentially meet project goals using database results and feedback from Carpenter



Summary



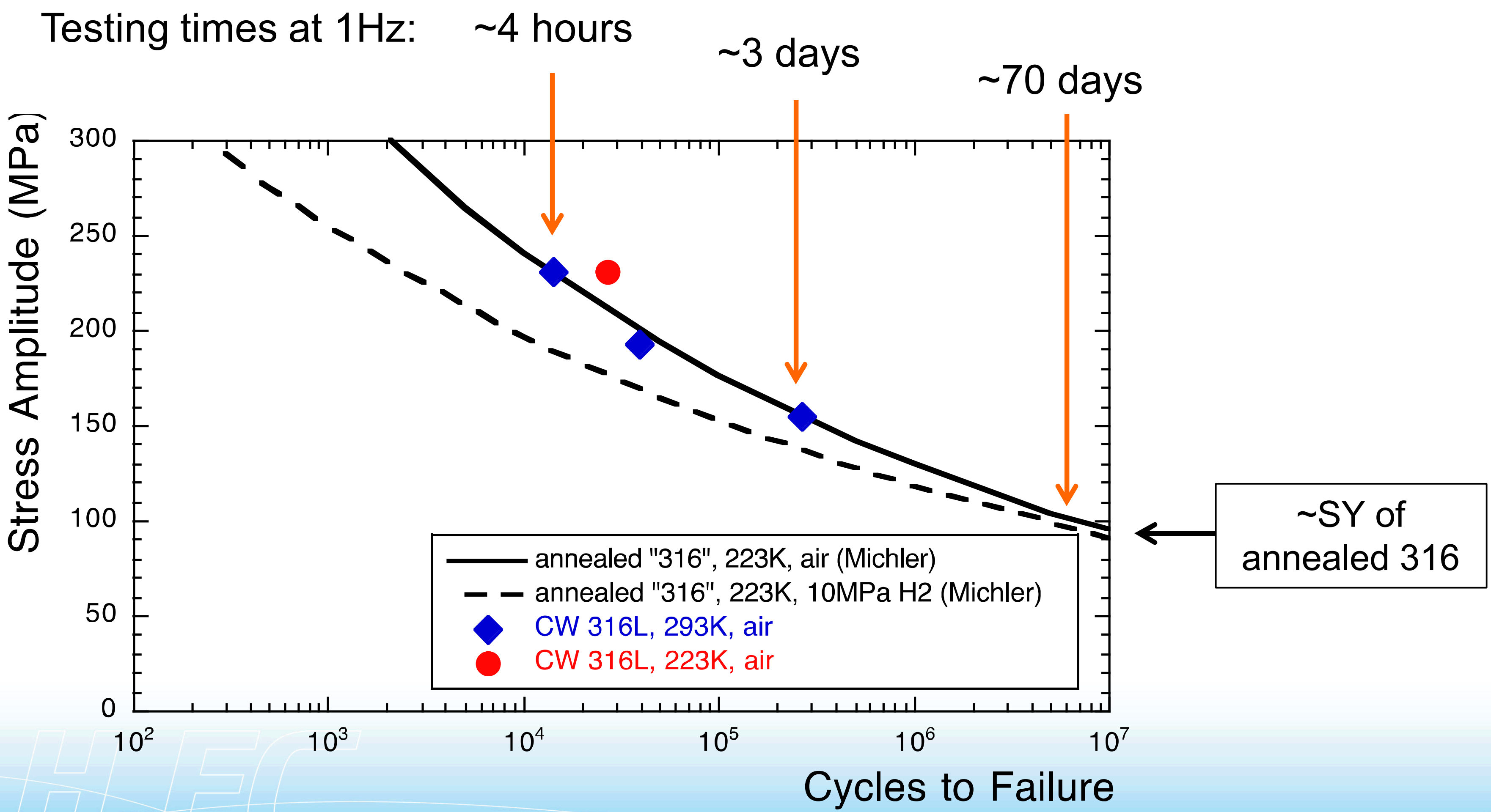
- "Back-of-the-envelope" calculations show large opportunity space for reducing cost and weight of materials for BOP
- Fatigue performance has been benchmarked with:
  - Notched tension-tension fatigue tests (CSA CHMC1)
  - High-strength type 316L with 12 wt% nickel
- Low-temperature fatigue performance suggests limiting behavior may be determined at room temperature for some alloys
- Methodology for *ab initio* determination of SFE is emerging
  - Ni supercell provides values consistent with literature
  - Minimum of 450 atoms per supercell are needed for Fe-Cr-Ni alloys
- TEM and extended fatigue analysis are anticipated to add value to understanding of behaviors and bridging observations at different length scales



Technical Back-Up Slides

(Note: please include this “separator” slide if you are including back-up technical slides (maximum of five). These back-up technical slides will be available for your presentation and will be included in the DVD and Web PDF files released to the public.)

Fatigue testing at low frequency requires long testing times



Reviewer-Only Slides

(Note: please include this "separator" slide between those to be presented and the "Reviewer-Only" slides. These slides will be removed from the presentation file and the DVD and Web PDF files.)

Response to Previous Year Reviewers' Comments

- This project was not reviewed last year

Critical Assumptions and Issues

- **Assumption**: SFE will be confirmed to be an appropriate metric for basing alloy optimization decisions based on relative value and ordering of SFE values for various alloy compositions with known or measured mechanical properties.
- **Issue**: If a correlation between SFE and mechanical properties is not confirmed, we will need to identify an alternative material property that's calculable from our *ab initio* approach would make for an appropriate descriptor, e.g. short range ordering, screw dislocation structure and cross slip behavior.

  Alternatively, DFT could be used to quantify how hydrogen and nitrogen exposure impact atomic-scale properties that do have relevance to plastic deformation, e.g. SFE. This result would provide insight on experimental findings within the project.

Publications and Presentations

- C. San Marchi and J.A. Zimmerman, X. Tang, S.J. Kernion, K. Thuermer, K.A. Nibur, “Fatigue life of austentic stainless steel in hydrogen environments” (PVP2015-45421), accepted for ASME 2015 Pressure Vessel and Piping Division Conference, Boston MA, 19-23 July 2015.
- C. San Marchi (presenter), “Hydrogen Energy Research at Sandia” (SAND2014-19188 PE), presented at SAE H2 Compatibility Workshop, 9 March 2015.
- C. San Marchi (presenter), “Innovative Development, Selection and Testing of Materials to Reduce Cost and Weight of BOP Components” (SAND2015- 1912 O), in-person presentation at Swagelok Company, 11 March 2015.