Development & Validation of Realistic Degradation Mode Models for the Waste Package and Drip Shield

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Nuclear Waste Technical Review Board (NWTRB)

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M&O Waste Package Operations

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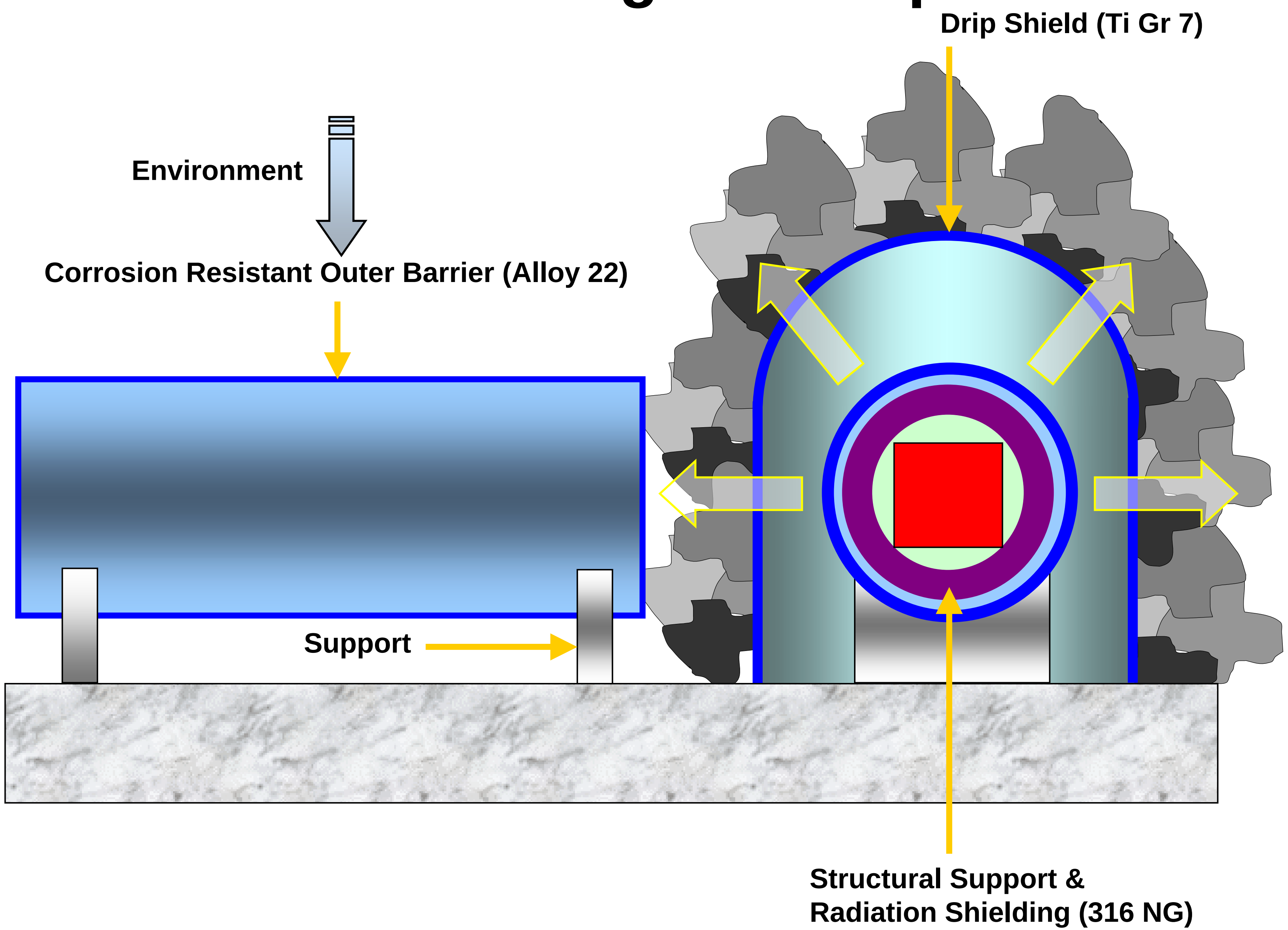
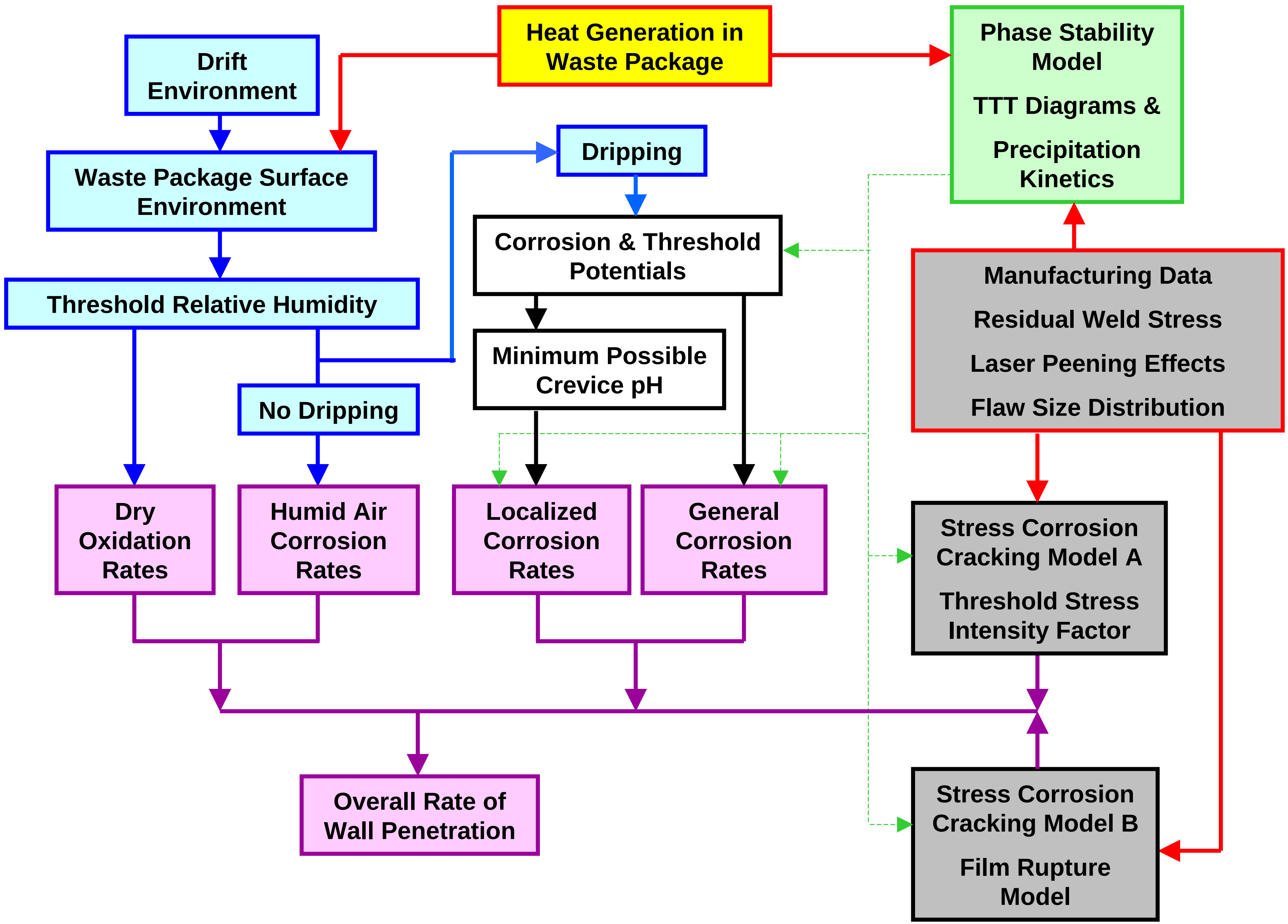
U.S. Department of Energy
Office of Civilian Radioactive
Waste Management

Yucca Mountain Project

Waste Package Concept



Abstracted Model for Waste Package Degradation

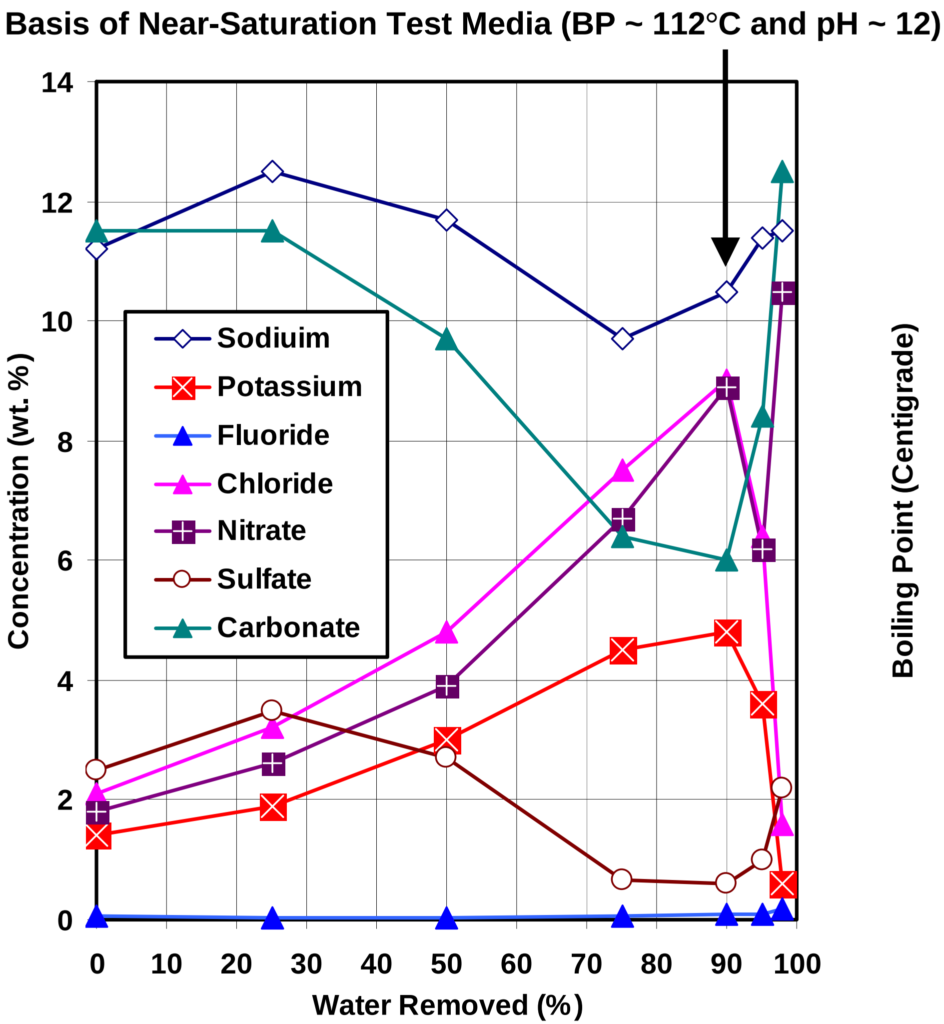


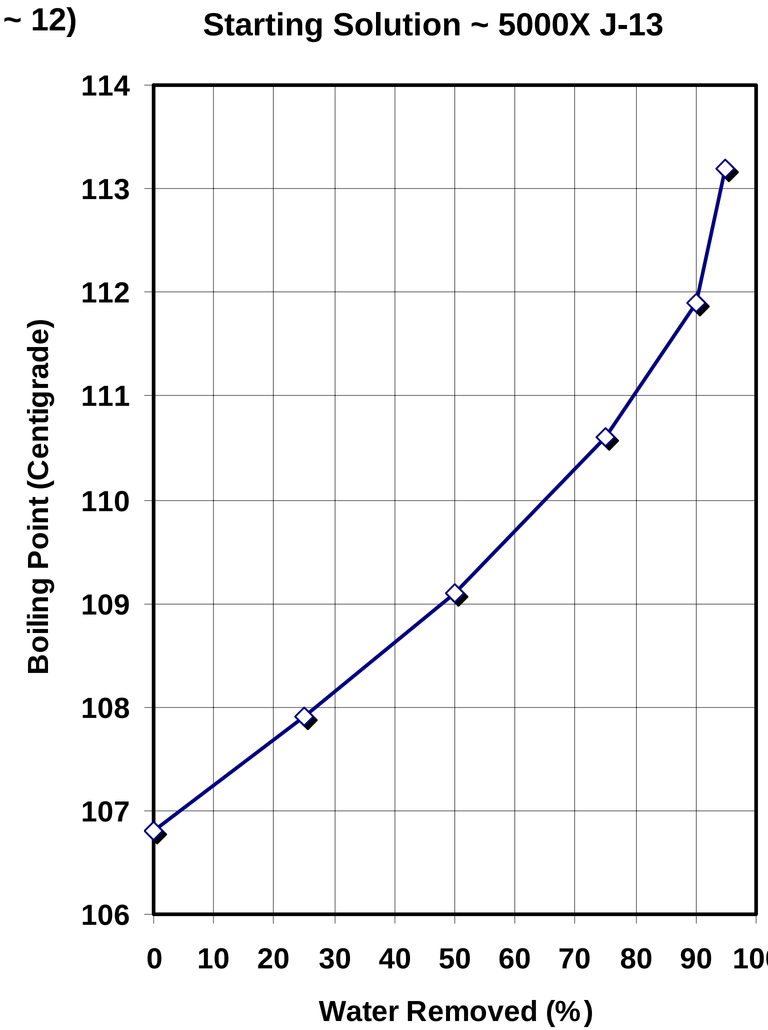
Examples of Model Validation

- **Validation is an essential part of model development**
  - **Corroboration with independent measurements**
  - **Bounding analyses**

- **Examples will be given relevant to the overall process model**
  - **General & Localized Corrosion**
    - **Weight loss measurements indicated very low corrosion rates**
    - **Cyclic polarization indicates very high thresholds potentials**
    - **Atomic Force Microscopy used for confirmation (validation)**
  - **Minimum Possible Crevice pH**
    - **Transport model used to predict low pH in crevice**
    - **Measurements and published data used to confirm predictions**
    - **Investigation of hydrogen absorption in titanium crevices**
  - **Stress Corrosion Cracking Models**
    - **Elimination of need through mitigation of weld stress**
  - **Aging & Phase Stability Model**
    - **Experimental validation with TEM & related techniques**

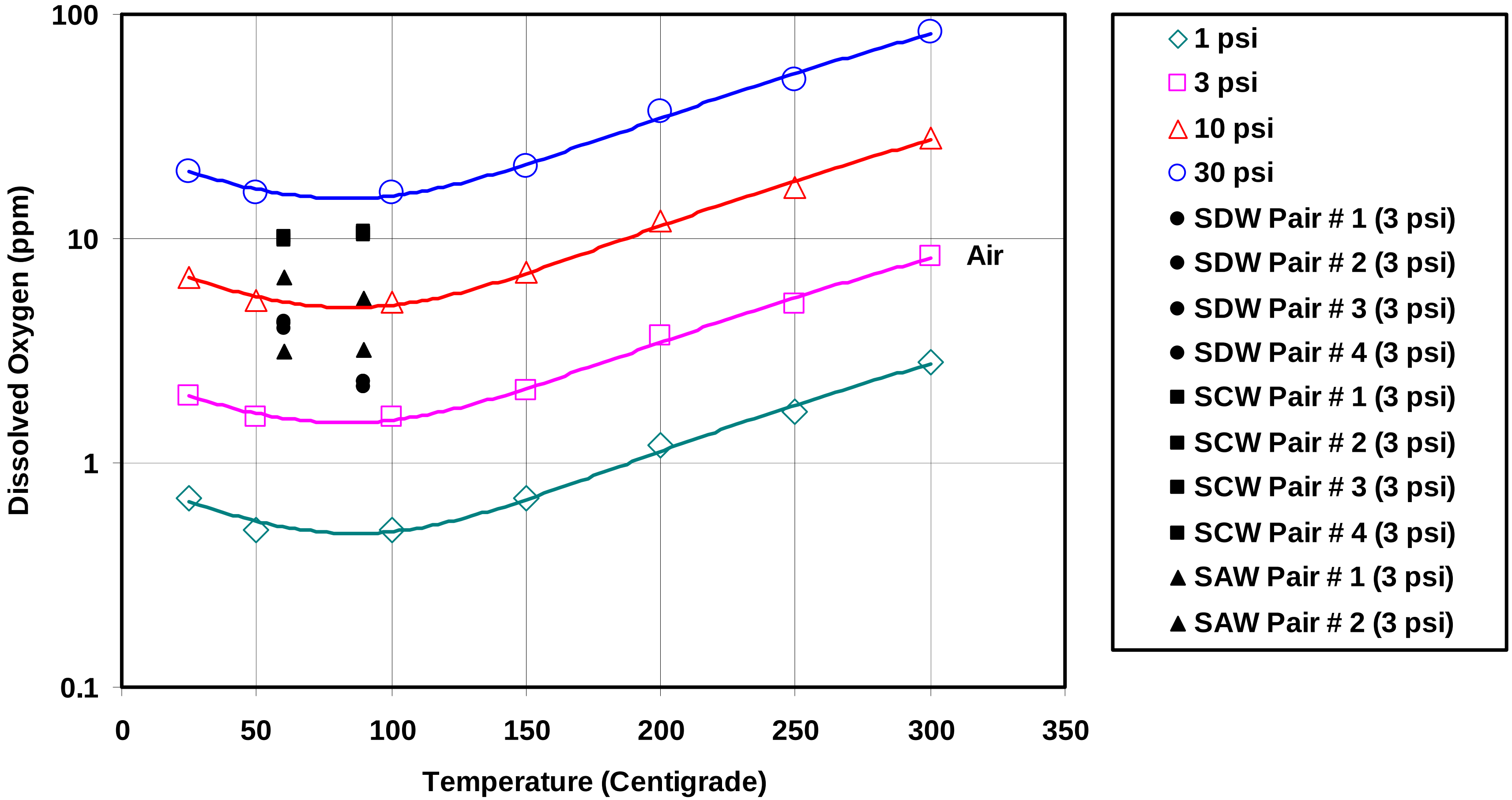
Establishment of New WP Surface Environment by Evaporative Concentration



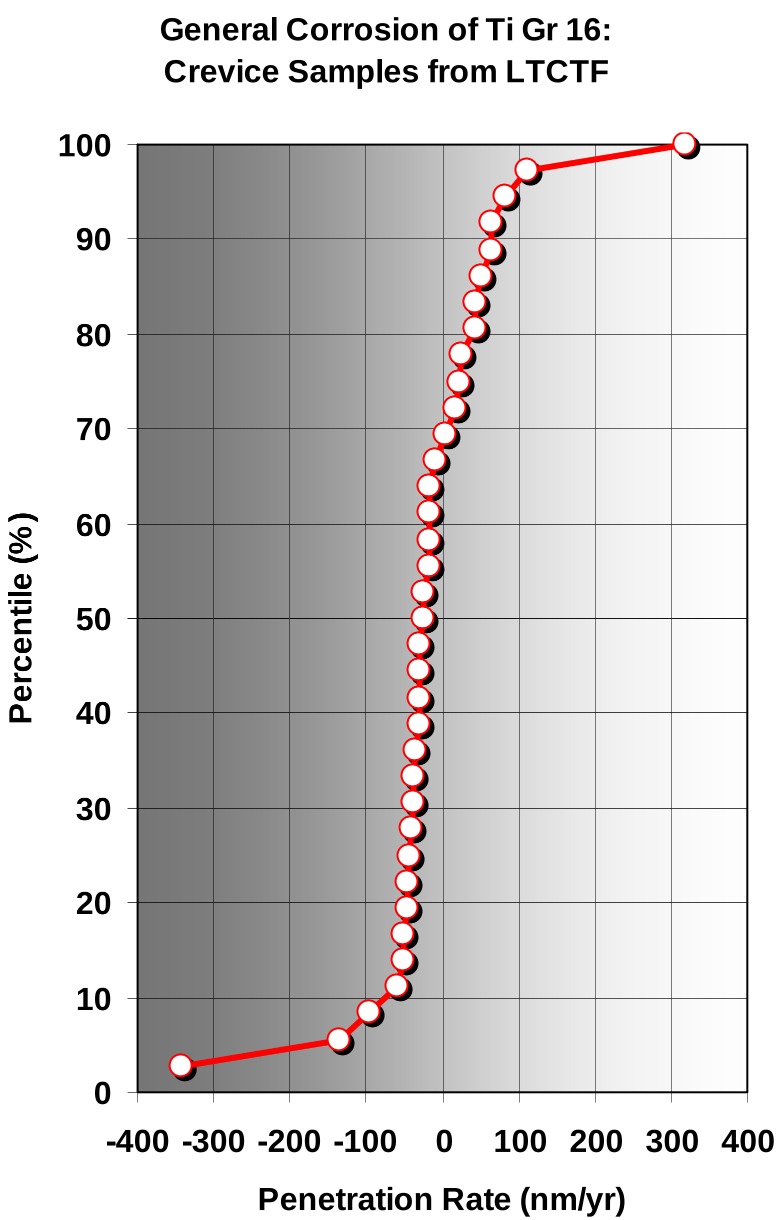


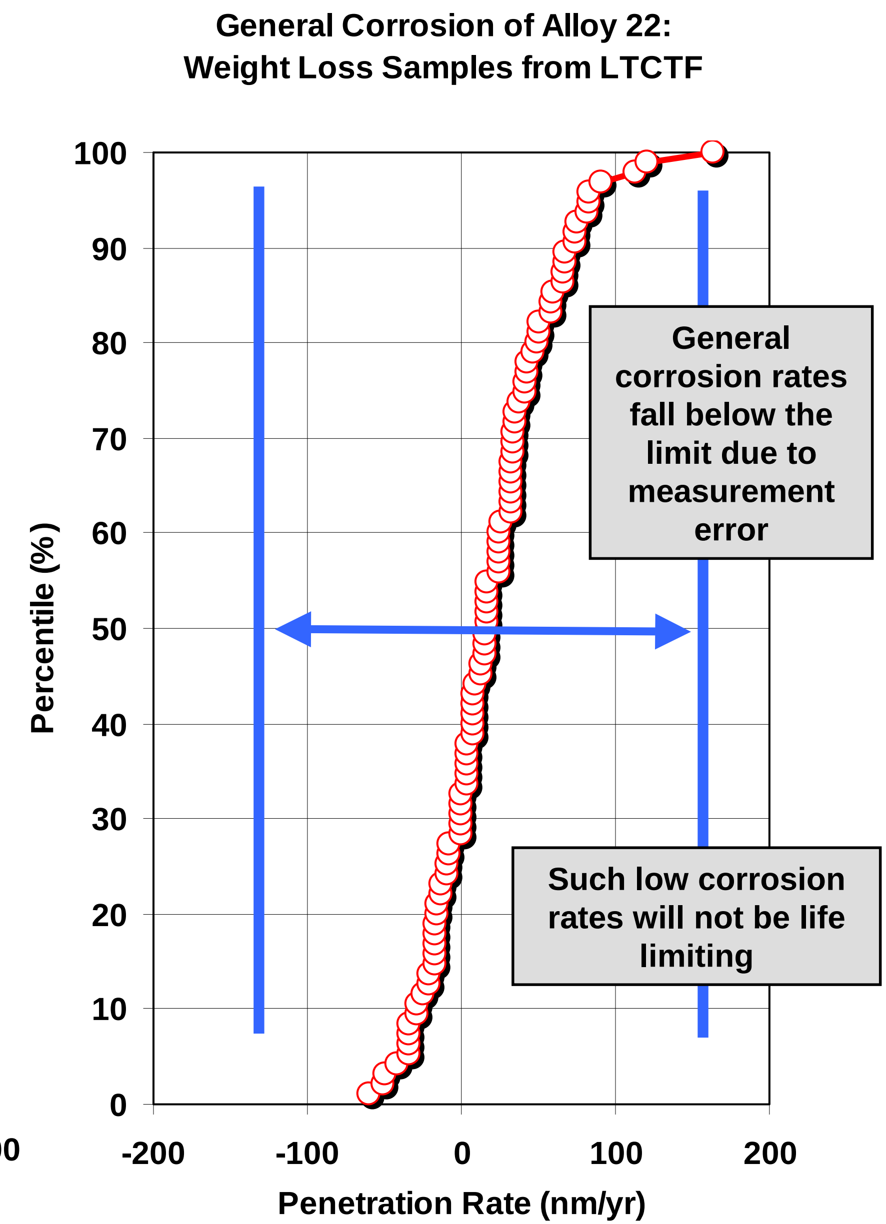
Since oxygen solubility (and corrosion rate) decreases with increasing salt concentration, the electrolyte formed by removing 90% of the water may be more severe than a fully saturated solution

Dissolved Oxygen Measurements in LTCTF Validated by Comparison to Published Data for Synthetic Geothermal Brine

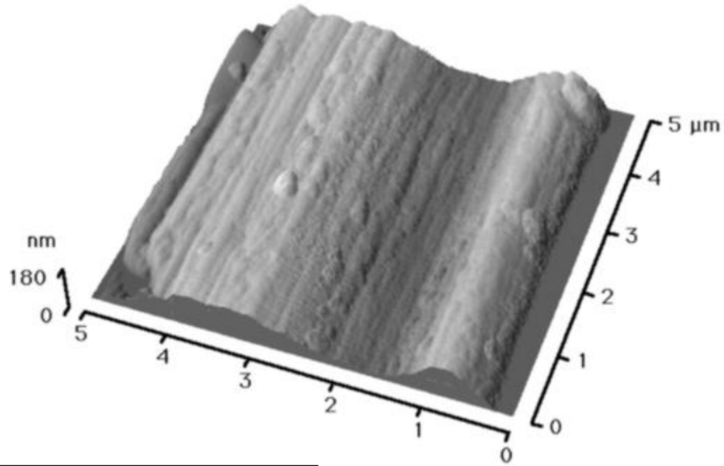


General Corrosion of DS & WP Materials

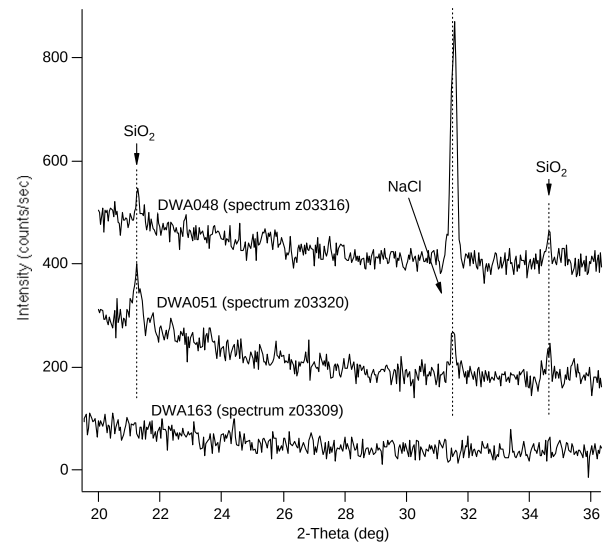




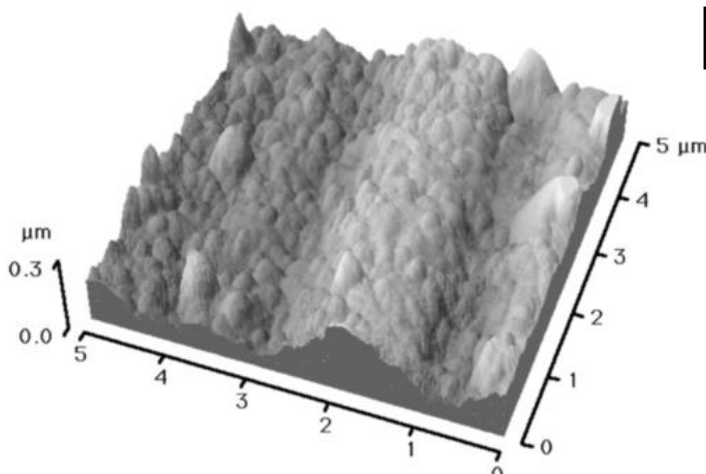
Low General Corrosion Rates Confirmed with AFM: Alloy 22 in LTCTF SAW at 90°C for 1 Year



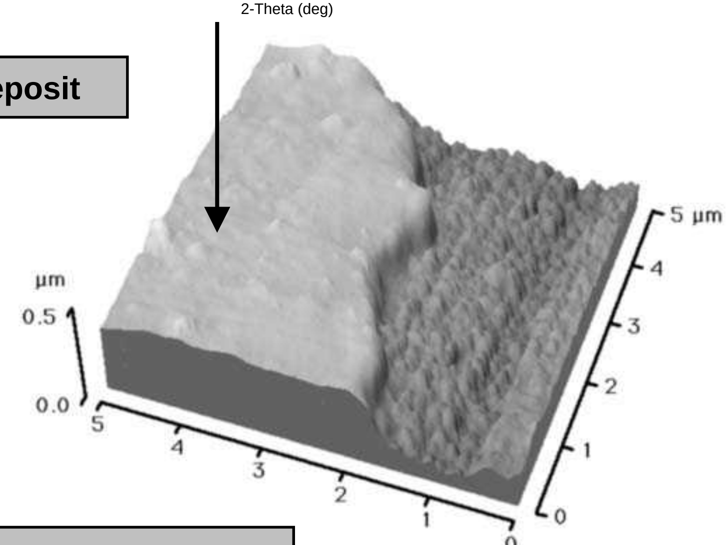
Control Sample



Silica Deposit



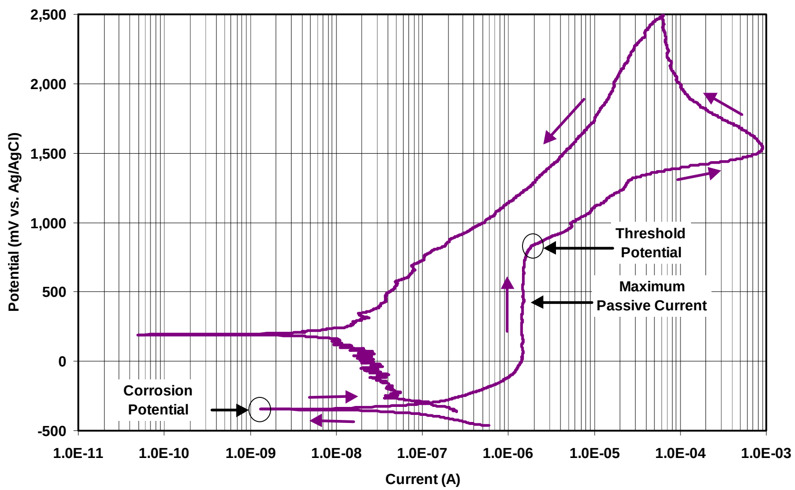
Vapor-Phase Exposure



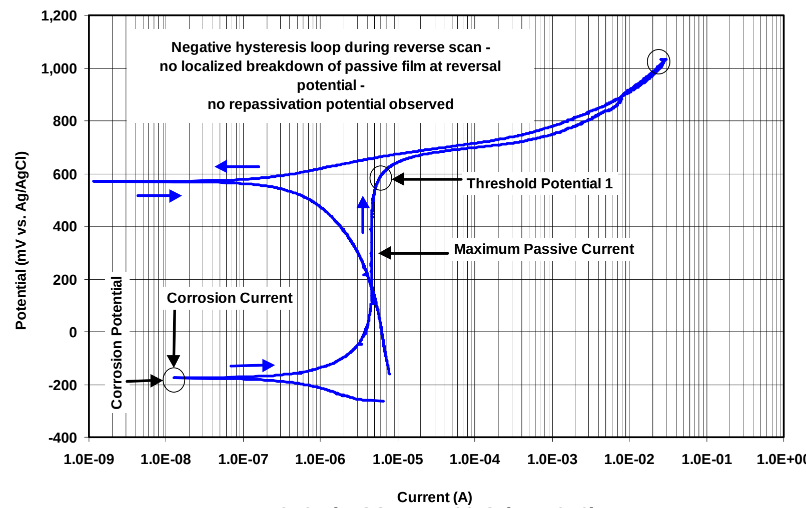
Liquid-Phase Exposure

DS & WP Resistant to Localized Corrosion

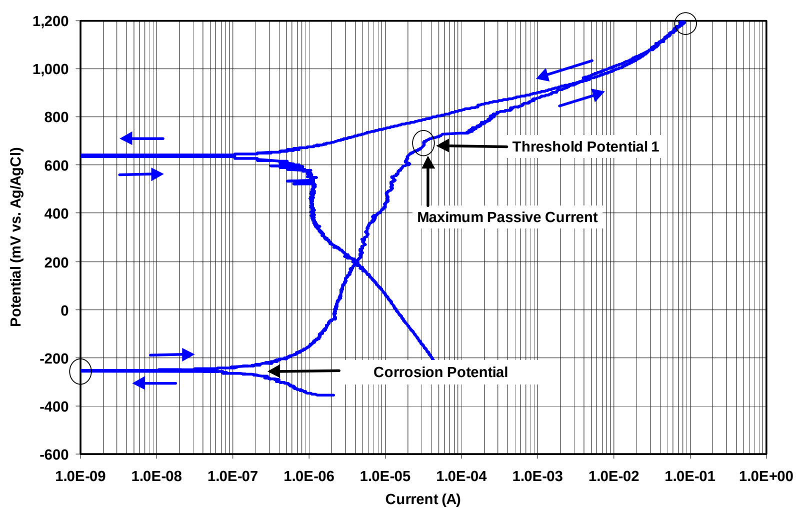
Ti Gr 7 in SSW at 120 C (NEA031s)



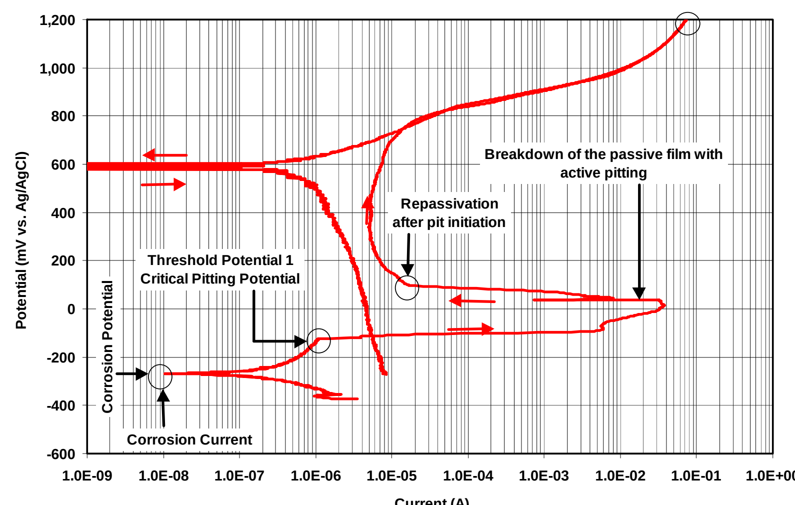
Alloy 22 in SAW at 90 C (DEA002)



Alloy 22 in SSW at 120 C (DEA033)



316L in SSW at 100 C (PEA016)

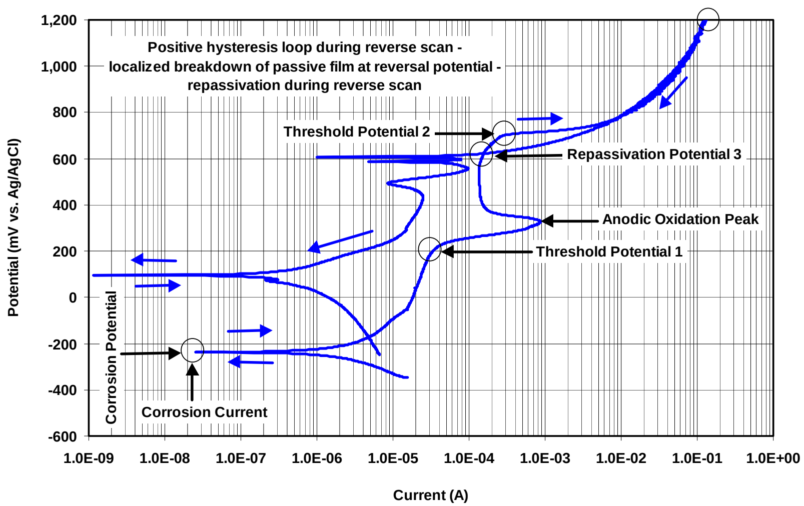


The DS & WP materials appear to have exceptional resistance to localized corrosion

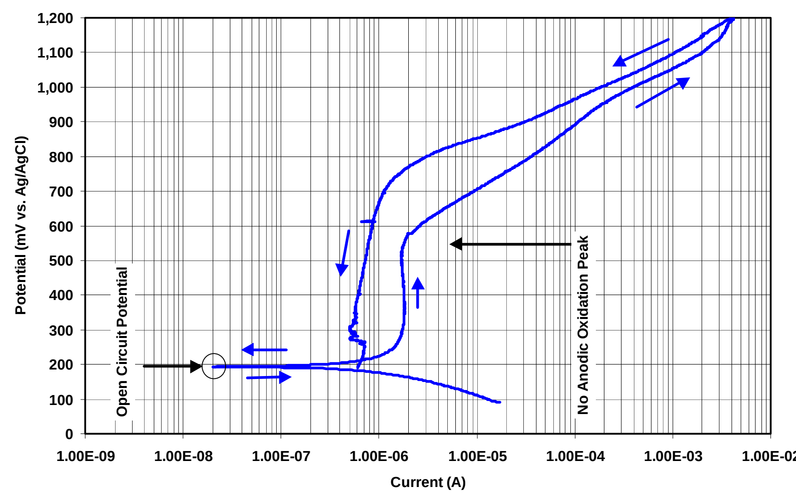
Stainless steel is to serve primarily as a structural material

Anodic Oxidation Peak with Alloy 22 in SCW

Alloy 22 in SCW at 90 C (DEA016)



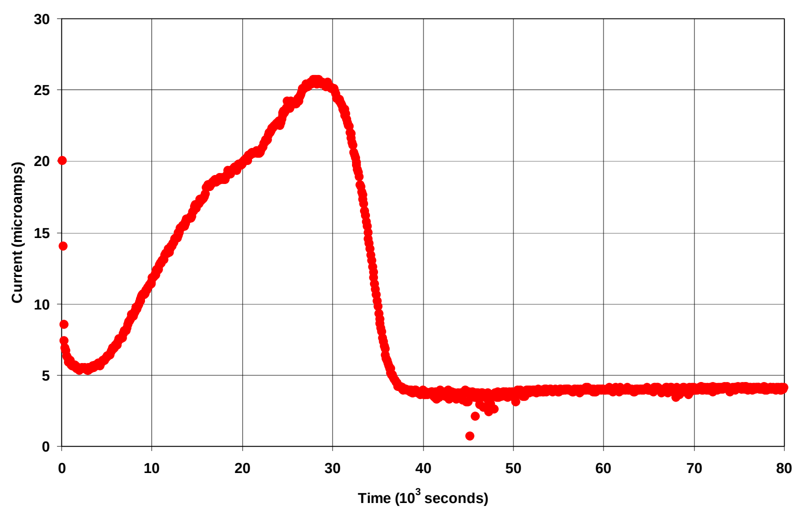
Baseline: Pt in SCW at 90 C (PT001)



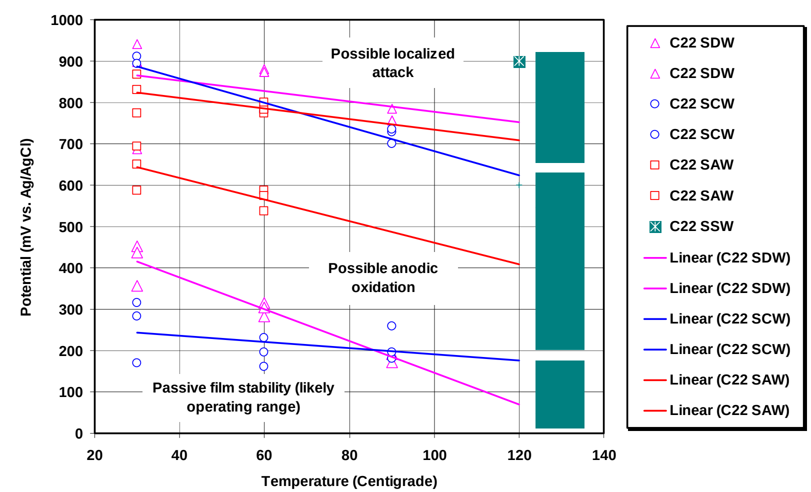
Anodic oxidation peaks observed in CP scans for Alloy 22 in SCW electrolytes

CP scans with Pt blank show that anodic peak due to surface phenomena

Potentiostatic Polarization of Alloy 22 in SCW at 90 C



Stability of Passive Film on Alloy C-22

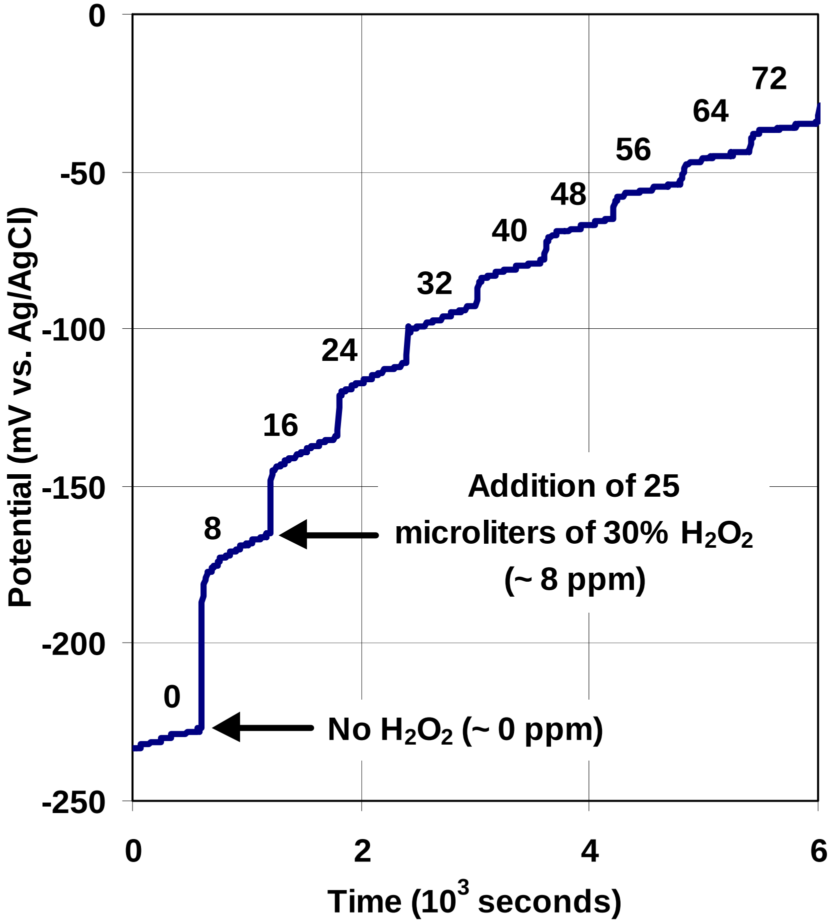


Gamma Radiolysis Effects: Insignificant Impact on Corrosion Potential & Breakdown of Passive Film

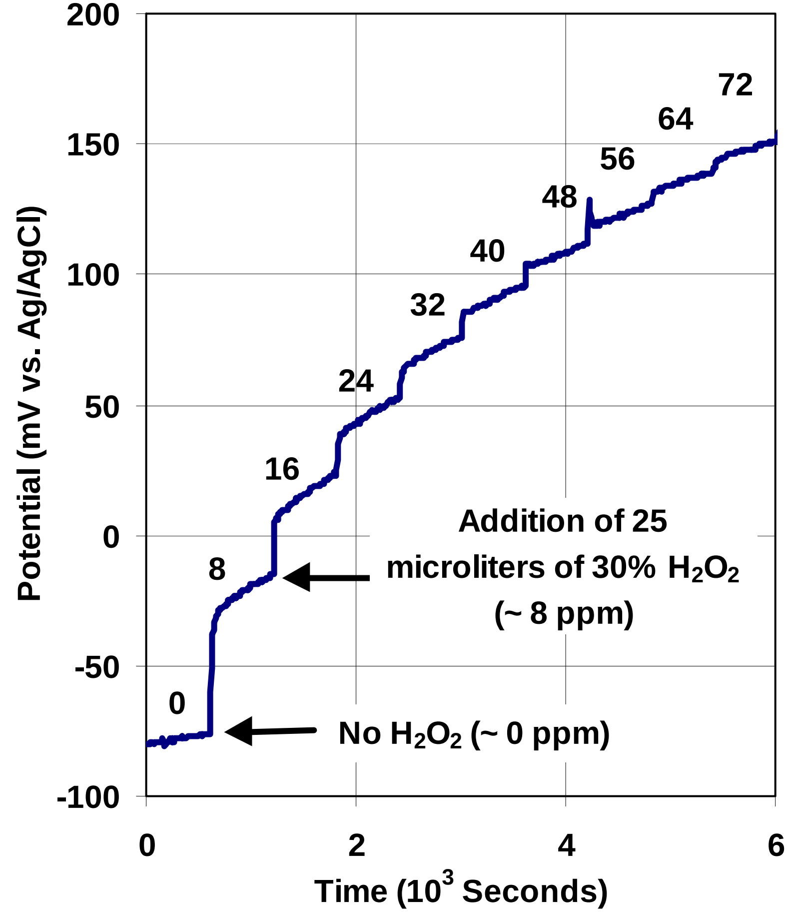
- **Gamma radiolysis could promote localized corrosion**
  - **Production of hydrogen peroxide**
  - **Anodic shift of the corrosion potential, closer to the threshold for breakdown of passive film**
- **A strategy has been formulated for addressing any enhanced radiolysis effects in the EDA II design**
  - **Re-examination stainless steel corrosion data from gamma pit that was produced by Yucca Mountain Project in the mid 1980's**
  - **Discussions with investigators at General Electric Corporation**
  - **Measurement of corrosion & threshold potentials of Alloy 22 and other WP materials as functions of H_2O_2 concentration**
- **Based upon such measurments, gamma radiolysis is being screened out as a signficant detrimental process**

Simulated Gamma Radiolysis Experiments with Alloy 22 in SCW and SAW

Effect of H_2O_2 on Corrosion Potential of Alloy 22 in SCW at 25 Centigrade



Effect of H_2O_2 on Corrosion Potential of Alloy 22 in SAW at 25 Centigrade



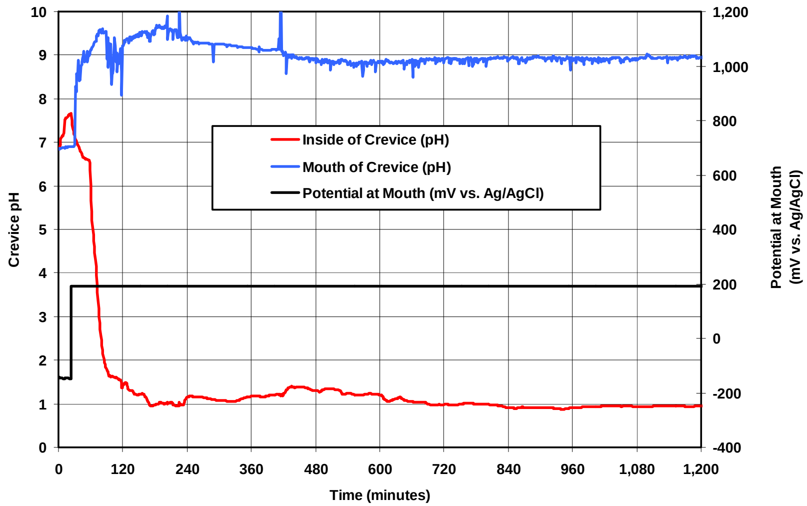
Hydrogen peroxide does not drive corrosion potential into anodic oxidation or regions of passive film destabilization in SAW or SCW

Minimum Possible Crevice pH

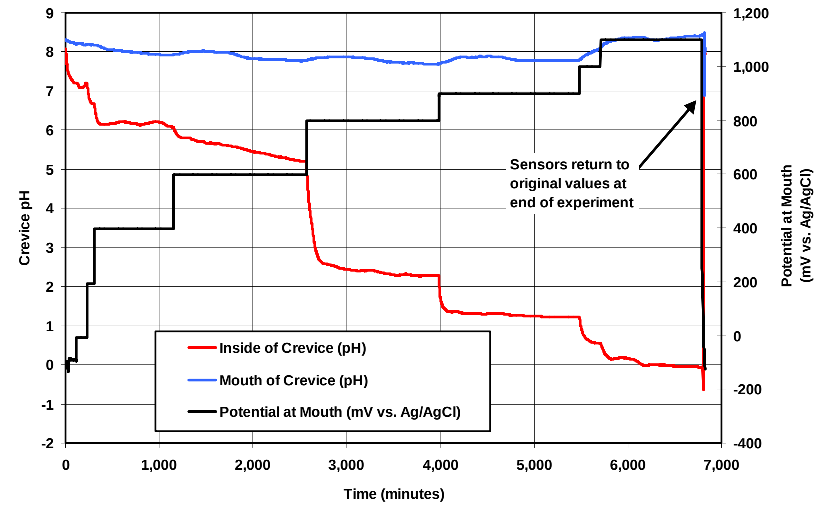
- **Crevices will be formed**
  - **Beneath mineral precipitates, corrosion products, dust, rocks, cement and biofilms**
  - **Between waste package and supports**
  - **Between outer barrier (Alloy 22) and inner barrier (316 NG)**
- **The crevice environment will be more severe than the NFE**
  - **Suppression of pH due to the accumulation of H^+ from the hydrolysis of dissolved metal**
  - **Field-driven electromigration of Cl^- (and other anions) into crevice must occur to balance cationic charge associated with H^+**
- **The crevice environment sets the stage for other modes of attack**
  - **General corrosion**
  - **Pitting (initiation & propagation)**
  - **Stress corrosion cracking (initiation & propagation)**
- **Successful defense of the Waste Package (WP) design requires adequate understanding of such phenomena**

Predicted Crevice Environment Confirmed with In Situ Measurments

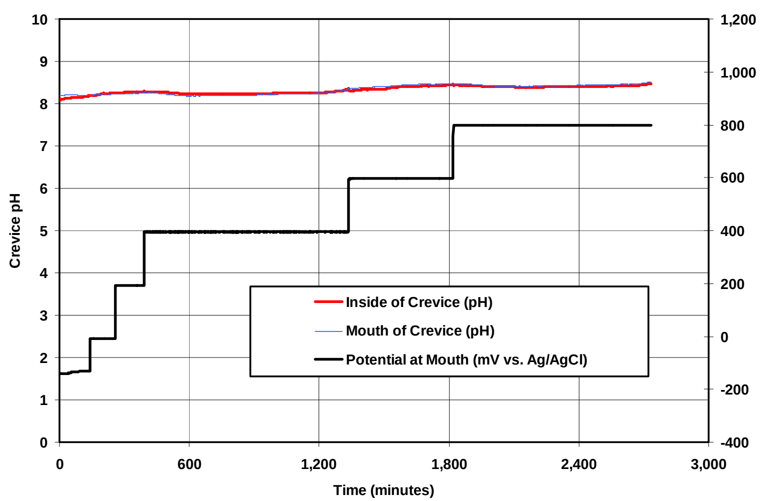
Stainless Steel 316L: 4M NaCl, 200 mV & 23 Centigrade



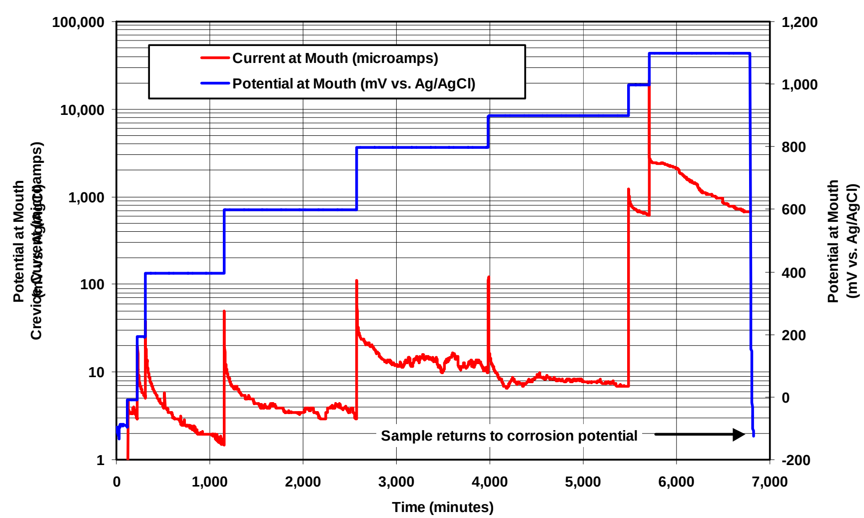
Alloy C-22 in 4M NaCl at 23 Centigrade



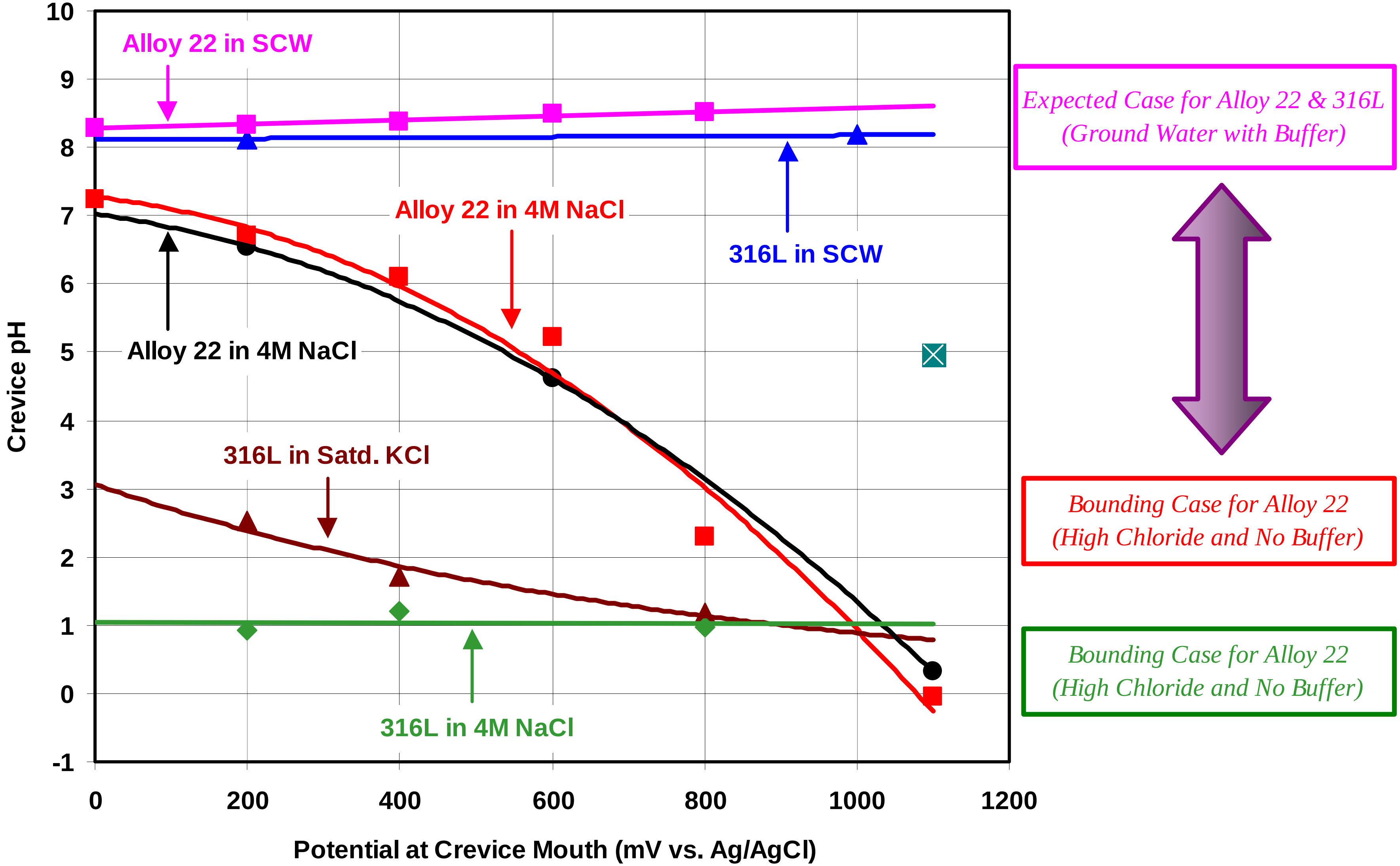
Alloy C-22 in SCW at 23 Centigrade



Alloy C-22 in 4M NaCl at 23 Centigrade

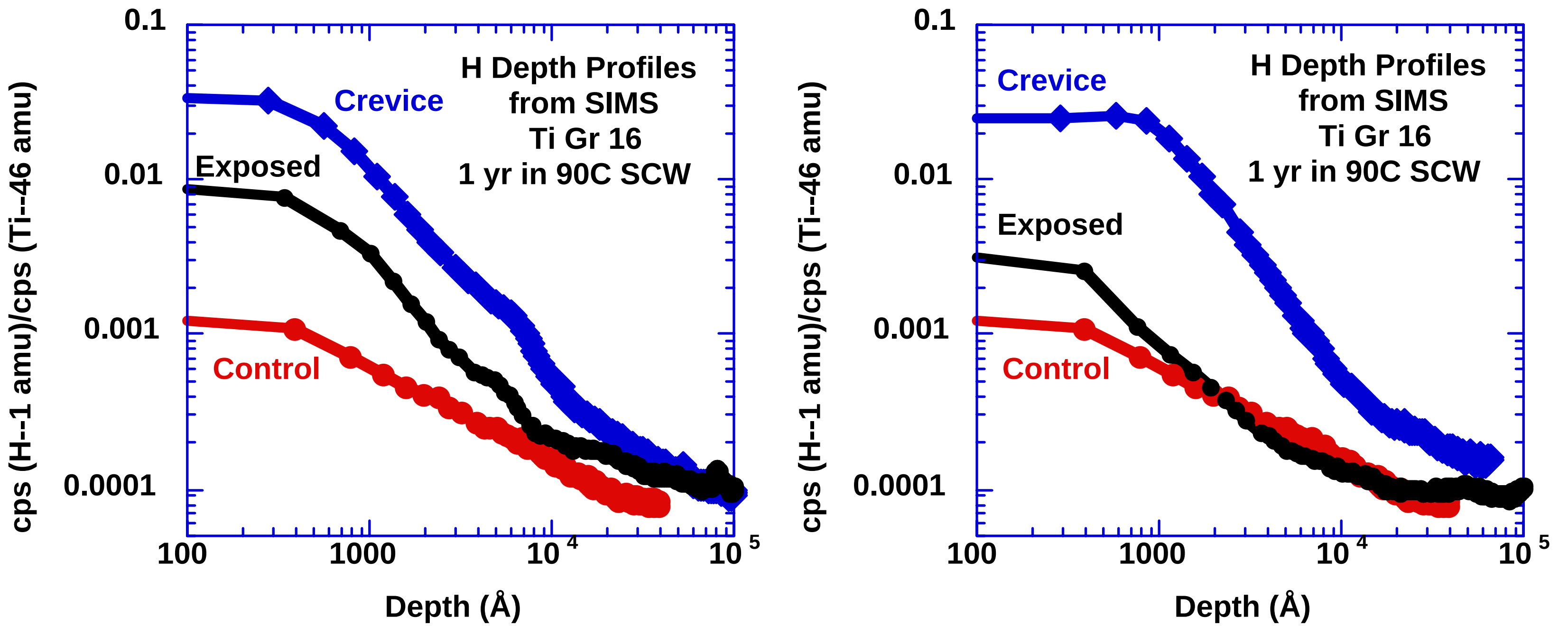


Determination of Crevice pH for WP Materials



Hydrogen Absorption in Titanium Crevice Confirmed with Secondary Ion Mass Spectrometry

SIMS Depth Profiles for Hydrogen

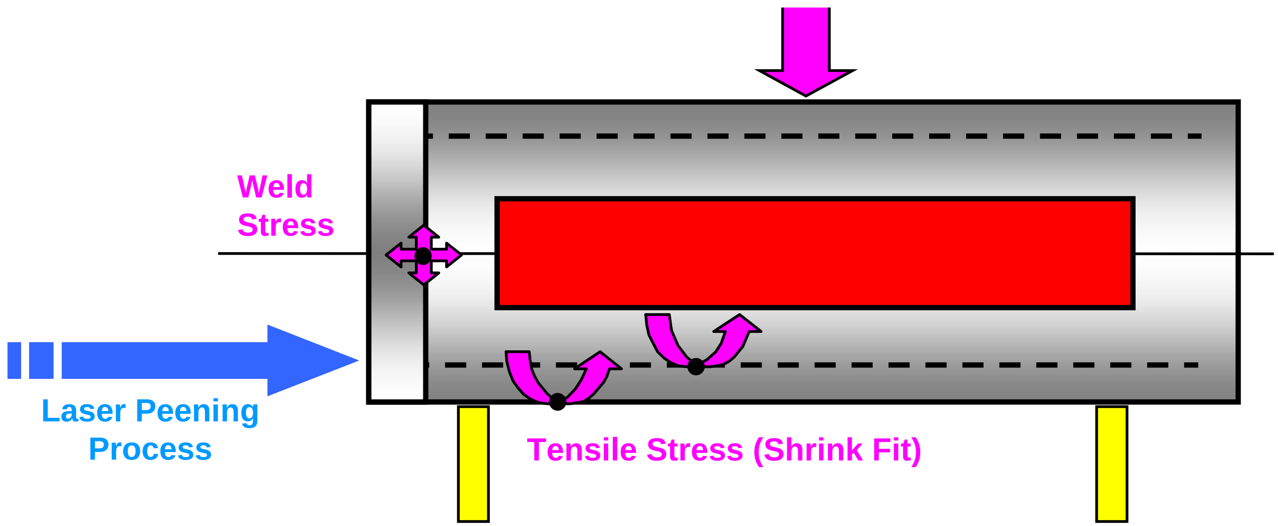


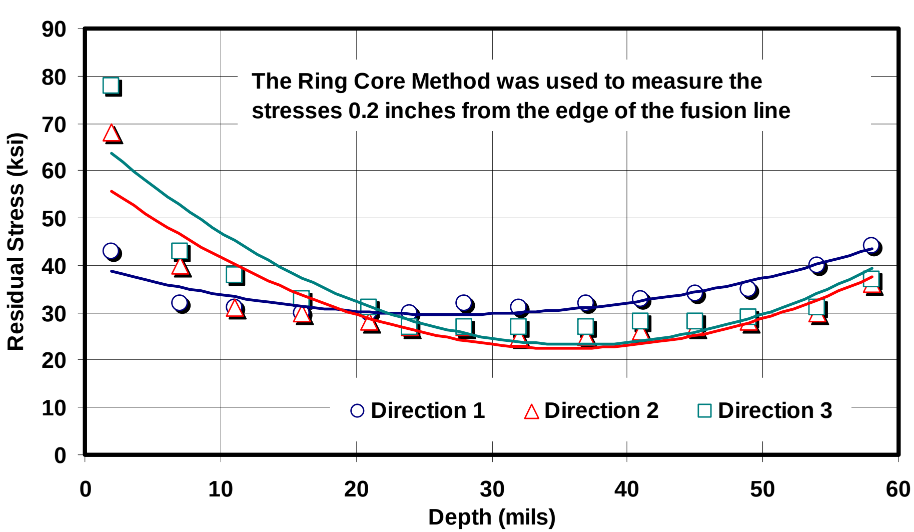
Hydrogen absorption by titanium is exacerbated by crevice. Additional work is needed to fully understand this phenomena. However, at the present time, it is not believed that the threshold hydrogen concentration for HIC will be exceeded.

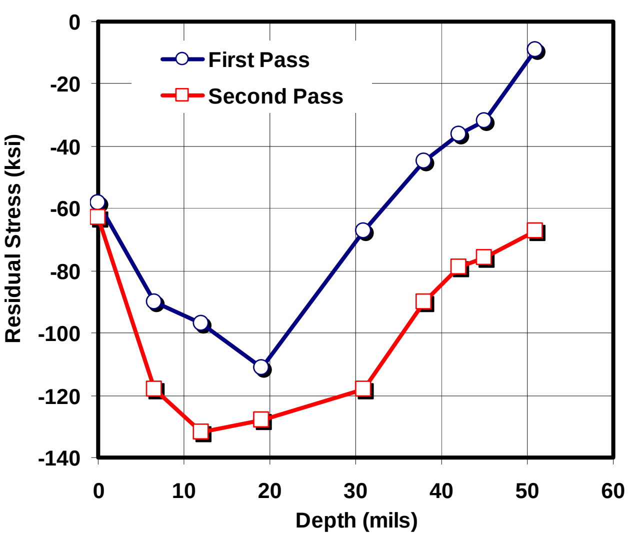
Validation of Stress Corrosion Cracking Models

- Slow strain rate testing
  - Experimental determination of stress-strain curves
  - Used for screening environment for other SCC tests
- Initiation based upon threshold stress intensity factor
  - Method employed by Yucca Mountain Project
  - Double Cantilever Beam Method (Ajit Roy)
  - Data have been obtained for Alloy 22 in NaCl solutions
- Finite propagation rate based upon film-rupture model
  - Method employed by General Electric Corporation
  - Reverse DC Method (Peter Andresen)
  - No data have been generated for Alloy 22
- Microbes may pose unique threats
  - Sulfate reducing bacteria (sulfide)
  - Iron oxidizing bacteria (ferric ion)

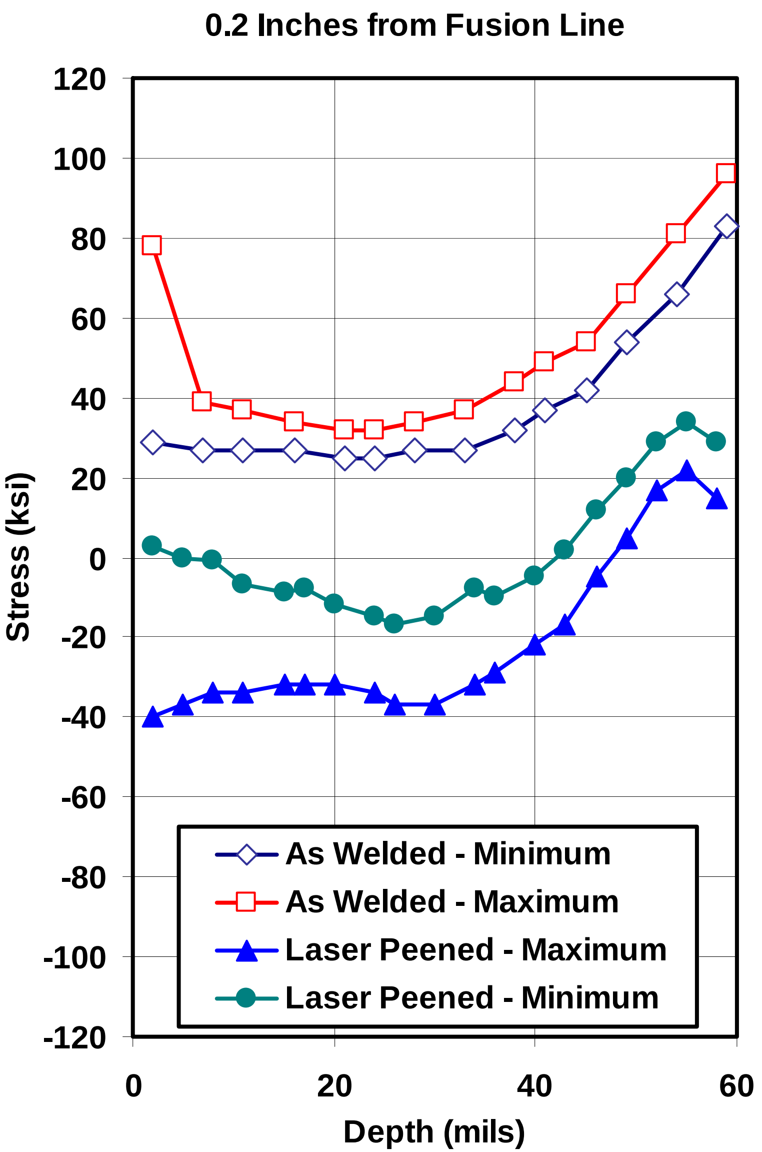
The Need for SCC Models Eliminated with Validated Technique for Stress Mitigation

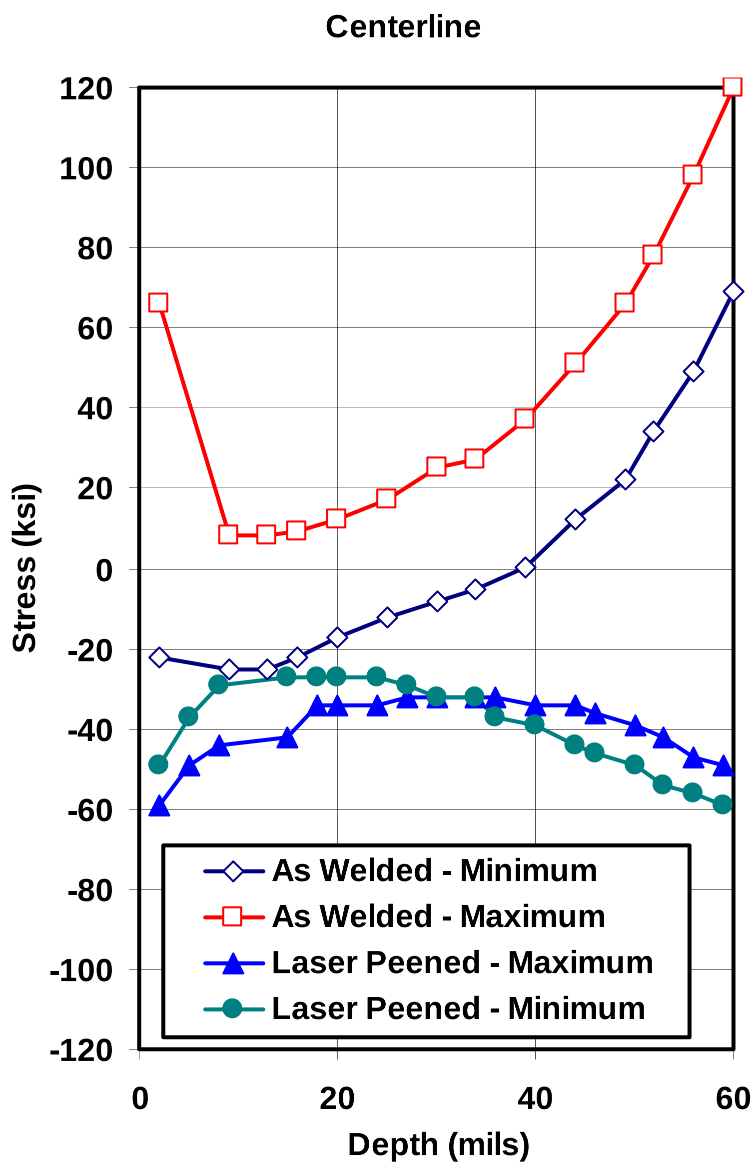






Mitigation of Weld Stress in Alloy 22 with Laser Peening

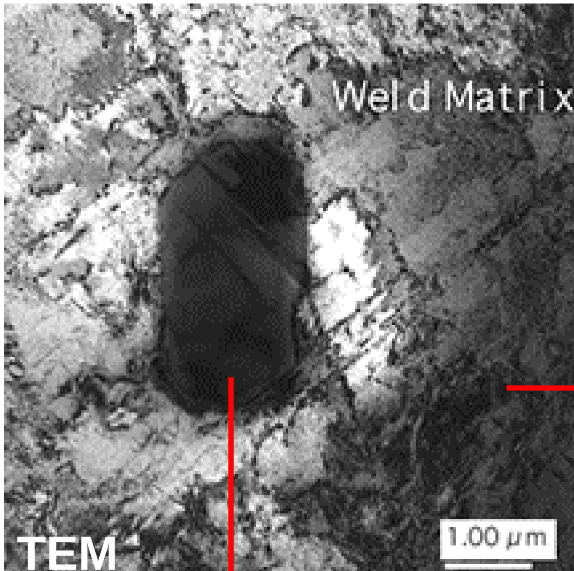


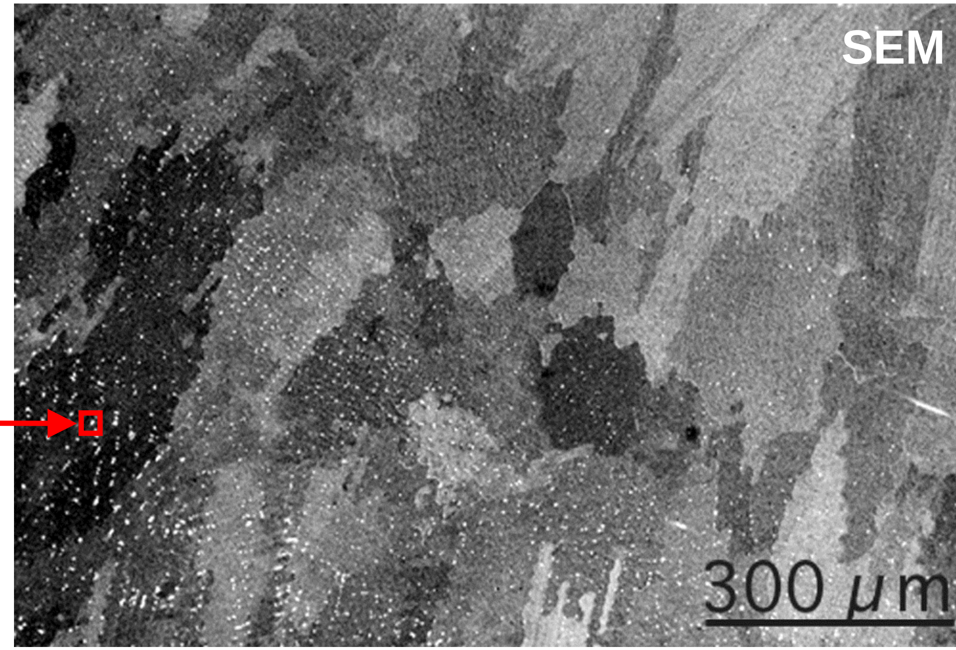


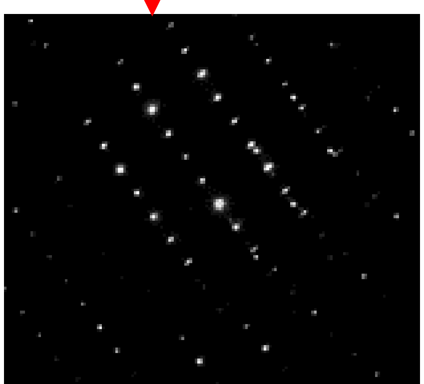
Theoretical Models for Aging & Phase Stability

- Theoretical tools and expertise are now in place to establish time-temperature-transformation (TTT) diagrams for multicomponent alloys
  — THERMO-CALC
  — DICTRA
- Phenomenological THERMO-CALC and DICTRA codes predict
  — Energetics
  — Regions of stability & metastability
  — Phase transformation rates limited by
    — Kinetics
    — Diffusive transport
- Electronic structure-based approach combined with Monte Carlo simulations used to
  — Supplement the thermodynamic databank
  — Predict solute effects on ordering processes, complex phase formation and evolution

Precipitated Intermetallic Phase Observed in Welded Alloy 22 Aged for 40,000 hr at 427°C



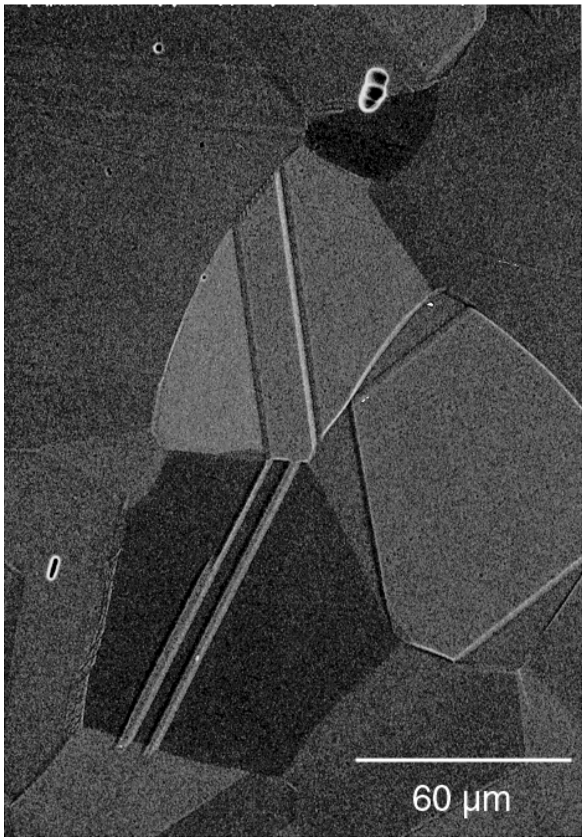




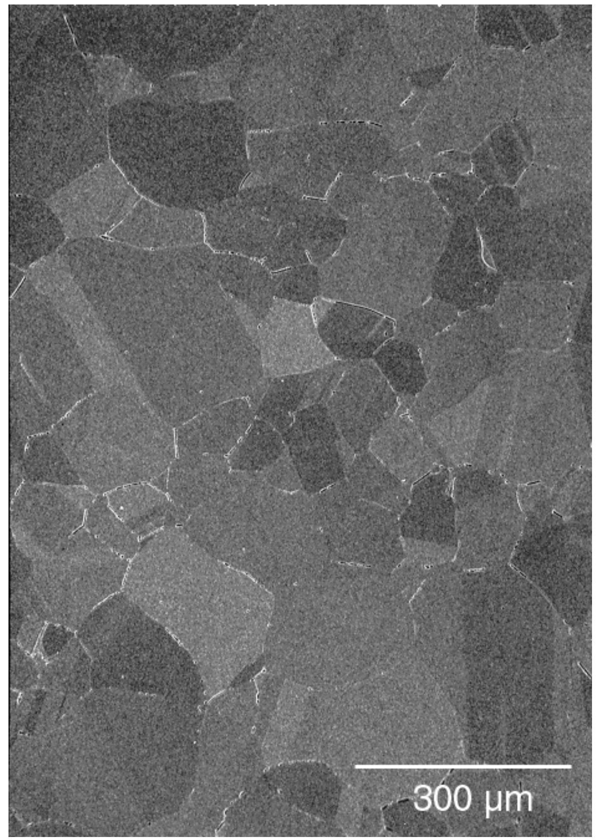
Theoretical models are being validated through detailed scientific research with transmission electron microscopy, electron beam diffraction, and other relevant techniques

Alloy C-22 Aged at 649 °C for Various Times

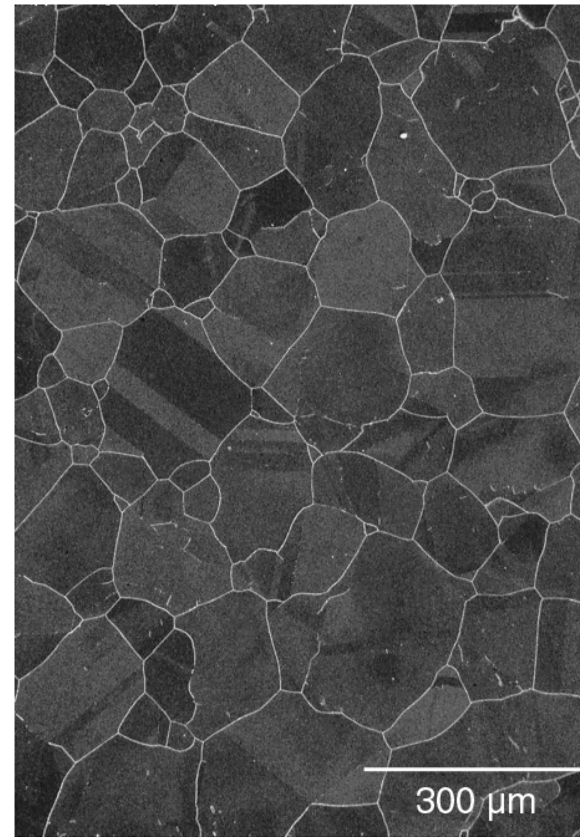
10 hr



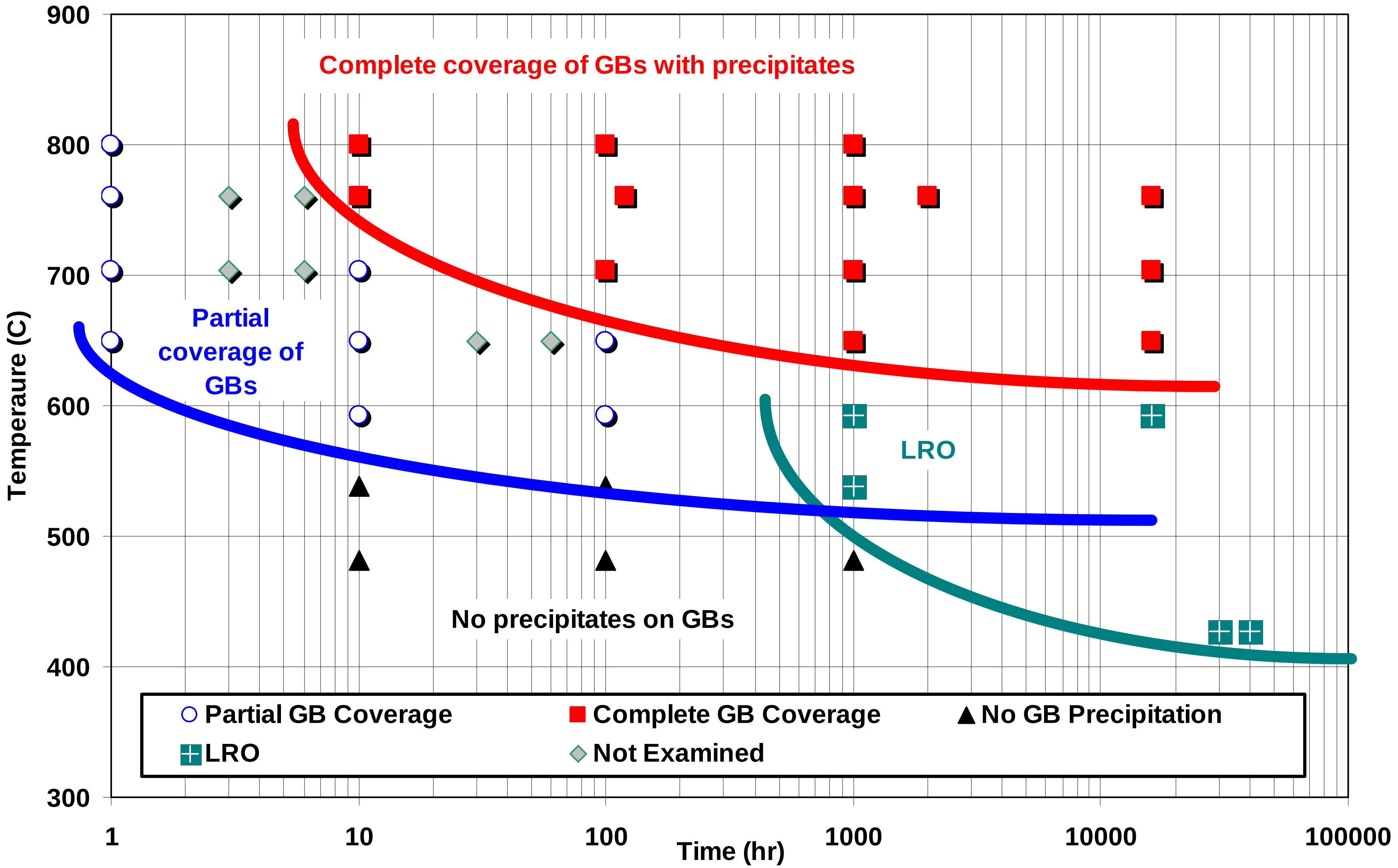
100 hr



1000 hr

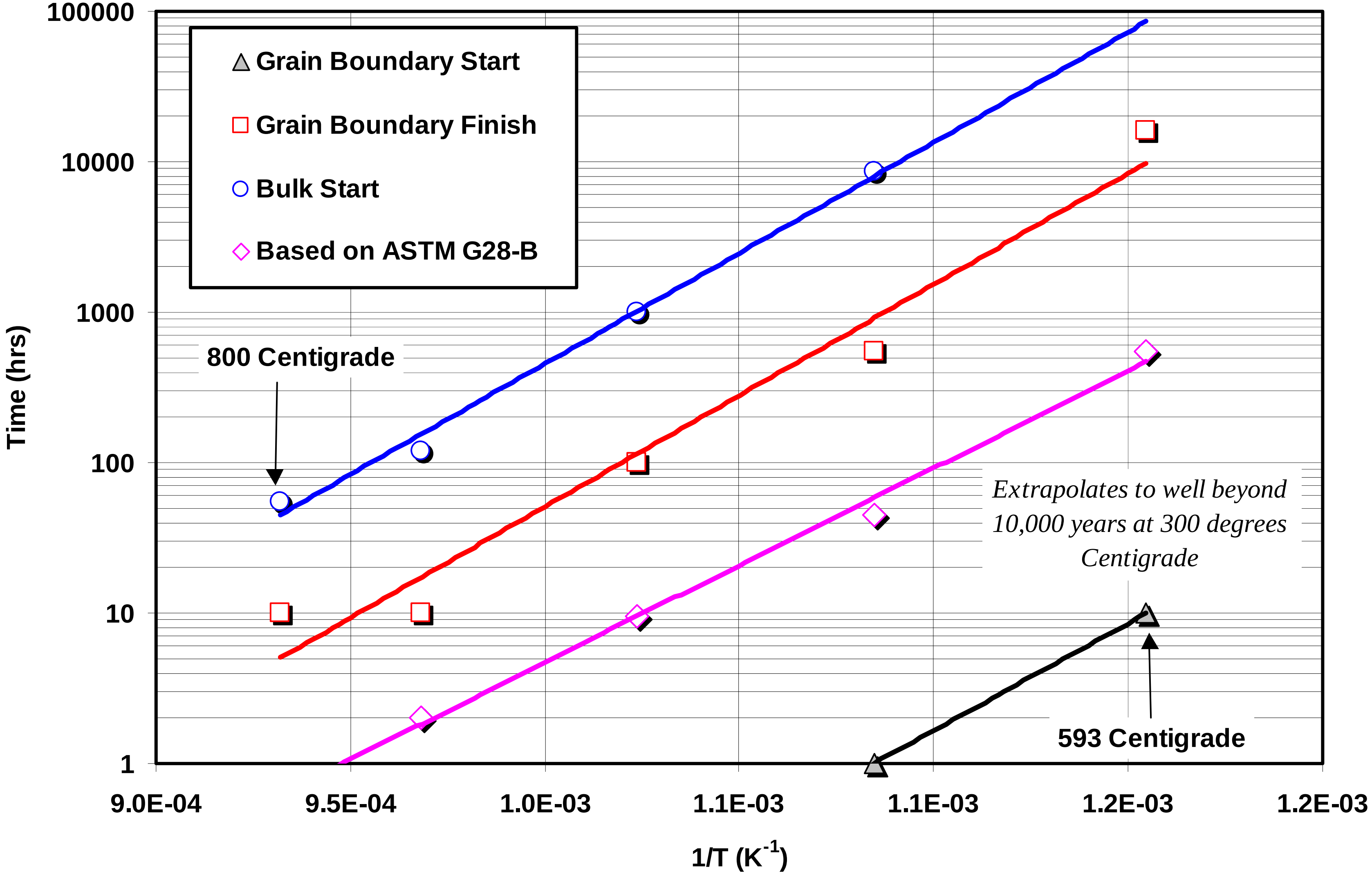


TTT Diagram for Alloy 22



Applicable to Base Metal

Preliminary Precipitation Kinetics for Alloy 22



Summary

- Validation is an essential part of model development
  - There are multiple ways to accomplish this
  - All have to be based upon good scientific investigation

- Examples will be given relevant to the overall process model
  - General & Localized Corrosion
    - Weight loss measurements indicated very low corrosion rates
    - Cyclic polarization indicates very high thresholds potentials
    - Atomic Force Microscopy used for confirmation (validation)
  - Minimum Possible Crevice pH
    - Transport model used to predict low pH in crevice
    - Measurements and published data used to confirm predictions
    - Investigation of hydrogen absorption in titanium crevices
  - Need for Stress Corrosion Cracking (SCC) model eliminated
    - Validation of new technique for mitigation of weld stress
  - Validation of Phase Stability Model

Summary

- **Preliminary conclusions**
  - — **No significant localized corrosion expected**
  - — **Life not limited by general corrosion**
  - — **Phase stability appears to be acceptable**
  - — **Focus on the mitigation of SCC at final closure weld**
- **New design has increased the need for additional testing**
  - — **Stainless steel & titanium were not used in TSPA-VA design**
  - — **Tests on these materials have just started**
  - — **Limited availability of qualified data**
- **Additional R&D must be directed towards fabrication processes**
  - — **Thermally enhanced fit of Alloy 22 outer barrier over 316NG**
    - — **Need to minimize tensile stress in Alloy 22 during cooling**
  - — **SCC threat at unannealed closure welds in Alloy 22**
    - — **Mitigation of through application of laser peening**

Valid WP Model Based Upon Contributions of Many

- **Definition of Interfacial Waste Package Environment**
  - **Greg Gdowski & Francis Wang**
- **Long Term Corrosion Testing**
  - **Dan McCright, John Estill, Ken King, Steve Gordon & Larry Logotetta**
- **Electrochemical Studies & Surface Physics**
  - **John Estill, Ken King, Steve Gordon & Larry Logotetta**
  - **Peter Bedrossian & David Fix**
- **Phase Stability**
  - **Tammy Summers, Patrice Turchi & Larry Kaufman**
- **Stress Corrosion Cracking Studies**
  - **Ajit Roy, John Estill, Maura Spragge, Dennis Fleming & Beverly Lum**
- **Microbial Influenced Corrosion**
  - **JoAnn Horn, Denny Jones & Tiangan Lian**
- **Welding Processes, Residual Stress Analysis & Laser Peening**
  - **Don Stevens, Lloyd Hackel, Fritz Harris (MIC) & Al Lingenfelter**
- **Waste Package Modeling**
  - **Patrice Turchi, Stephen Lu, & Jia-Song Huang**