Bespoke Materials Surfaces

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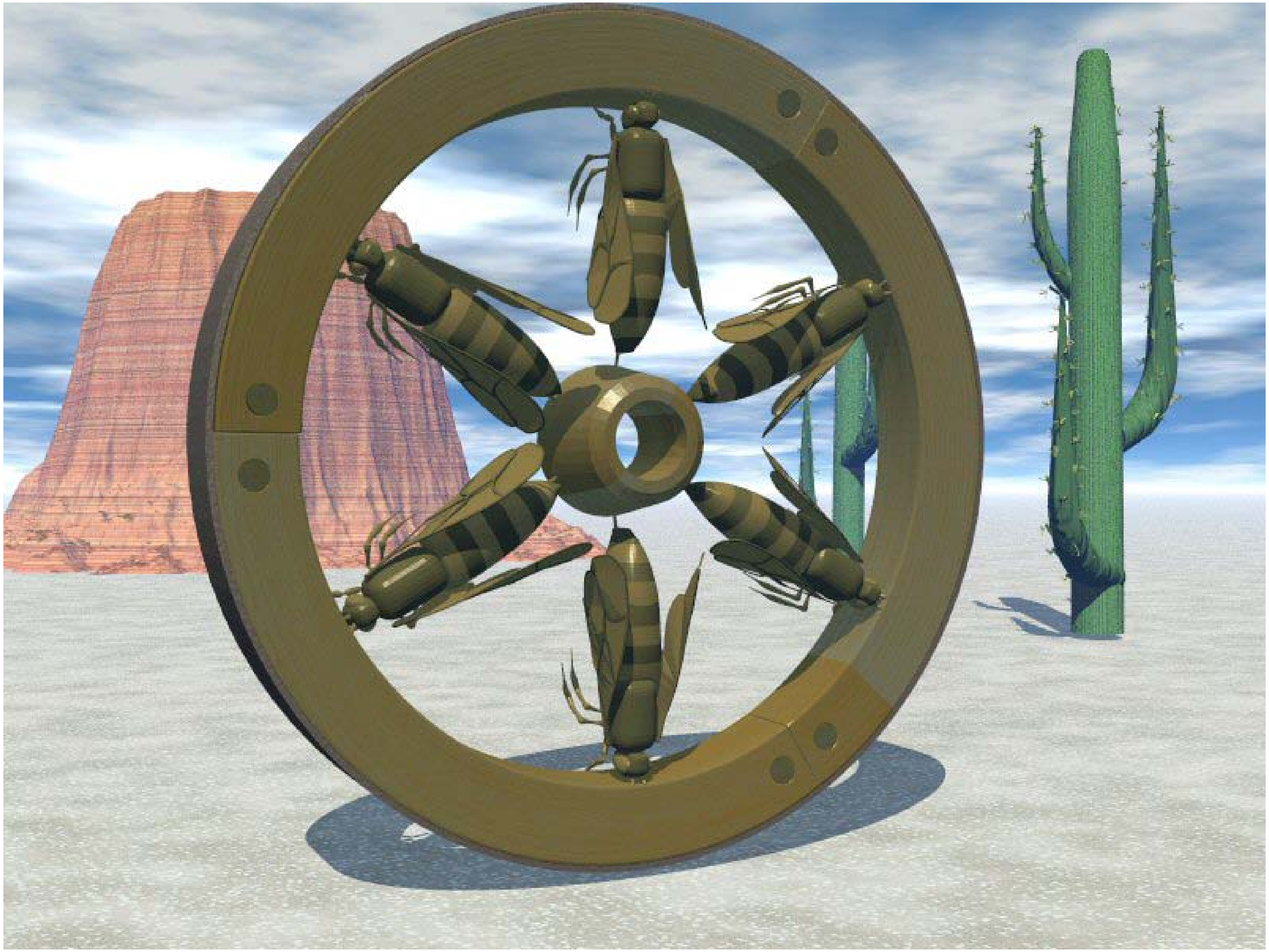
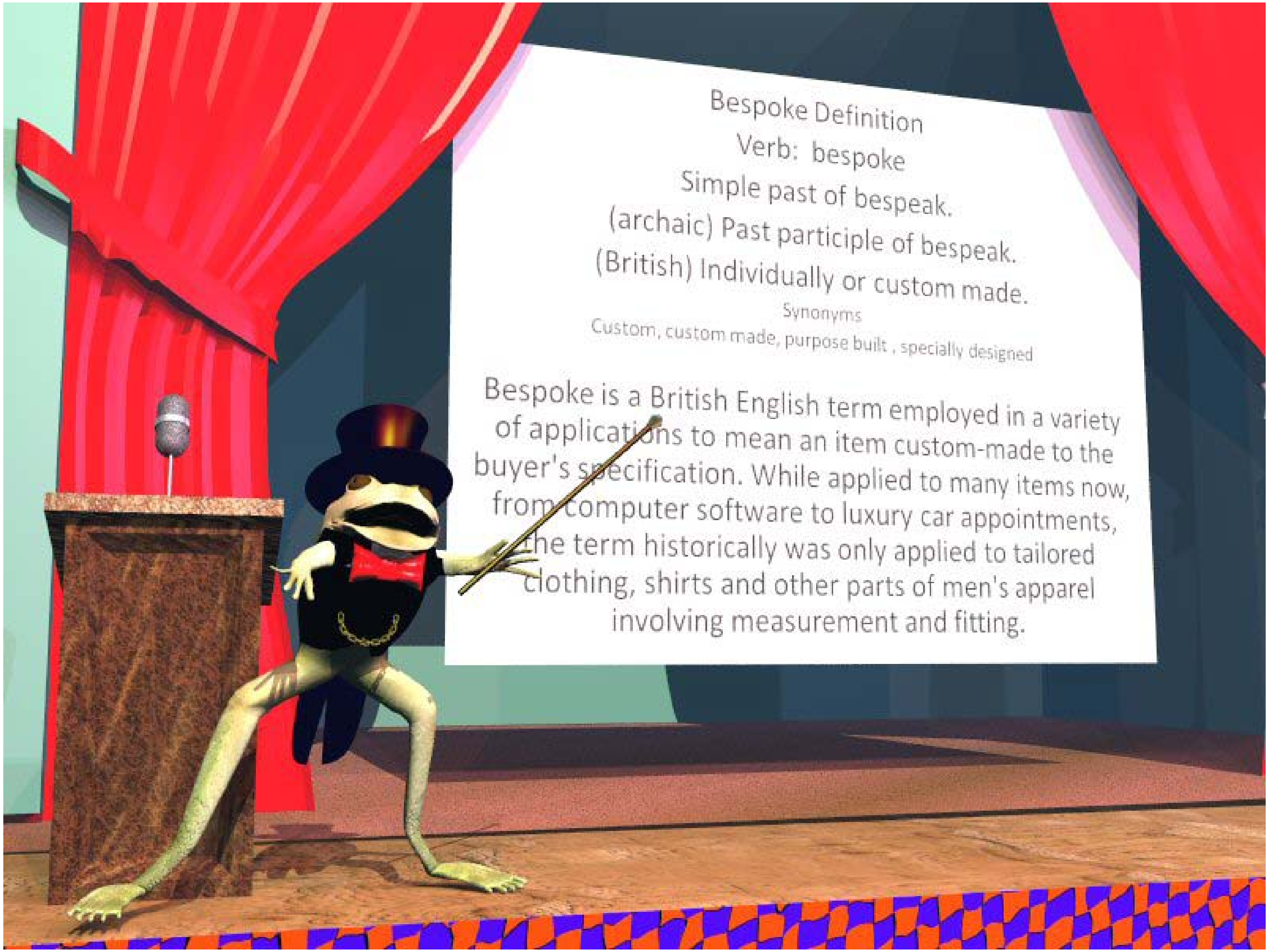
Bespoke…. A New Start Project, But What Does It Mean? Bee spokes



Bespoke…. Bees poke

Bespoke…. Tailored



Bespoke Definition
Verb: bespoke
Simple past of bespeak.
(archaic) Past participle of bespeak.
(British) Individually or custom made.
Synonyms
Custom, custom made, purpose built , specially designed

Bespoke is a British English term employed in a variety of applications to mean an item custom-made to the buyer's specification. While applied to many items now, from computer software to luxury car appointments, the term historically was only applied to tailored clothing, shirts and other parts of men's apparel involving measurement and fitting.

Outline

- Background: Advanced materials for fireside fossil energy applications
- Problem: Corrosion and thermal fatigue of coal-fired boiler waterwall tubes
- Objective: Develop material surfaces that have good adherence, high resistance to fireside corrosion/sulfidation, limited effect on thermal conductivity, are easy to apply
- Approach
    - Modeling of properties/identification of materials
    - Surface modifications/coatings
    - Testing
- Research Highlights
- Future Research
- Acknowledgements

Advanced Materials for Fireside Fossil Energy Applications

- Temperatures up to 900 ºC
- Aggressive species include:
  - Sulfur
  - Steam
  - Alkalis
  - High and low pO_2
  - Ash
- Thermal fatigue cracking
- The efforts in this project are aimed at developing a cost effective process for engineering protective surfaces

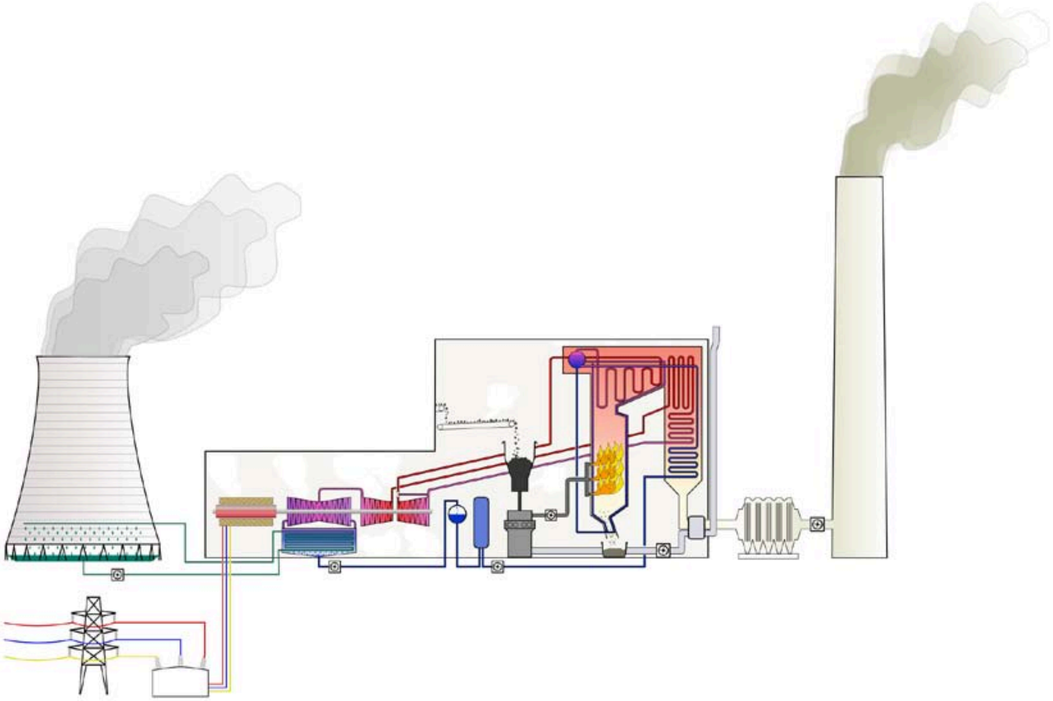
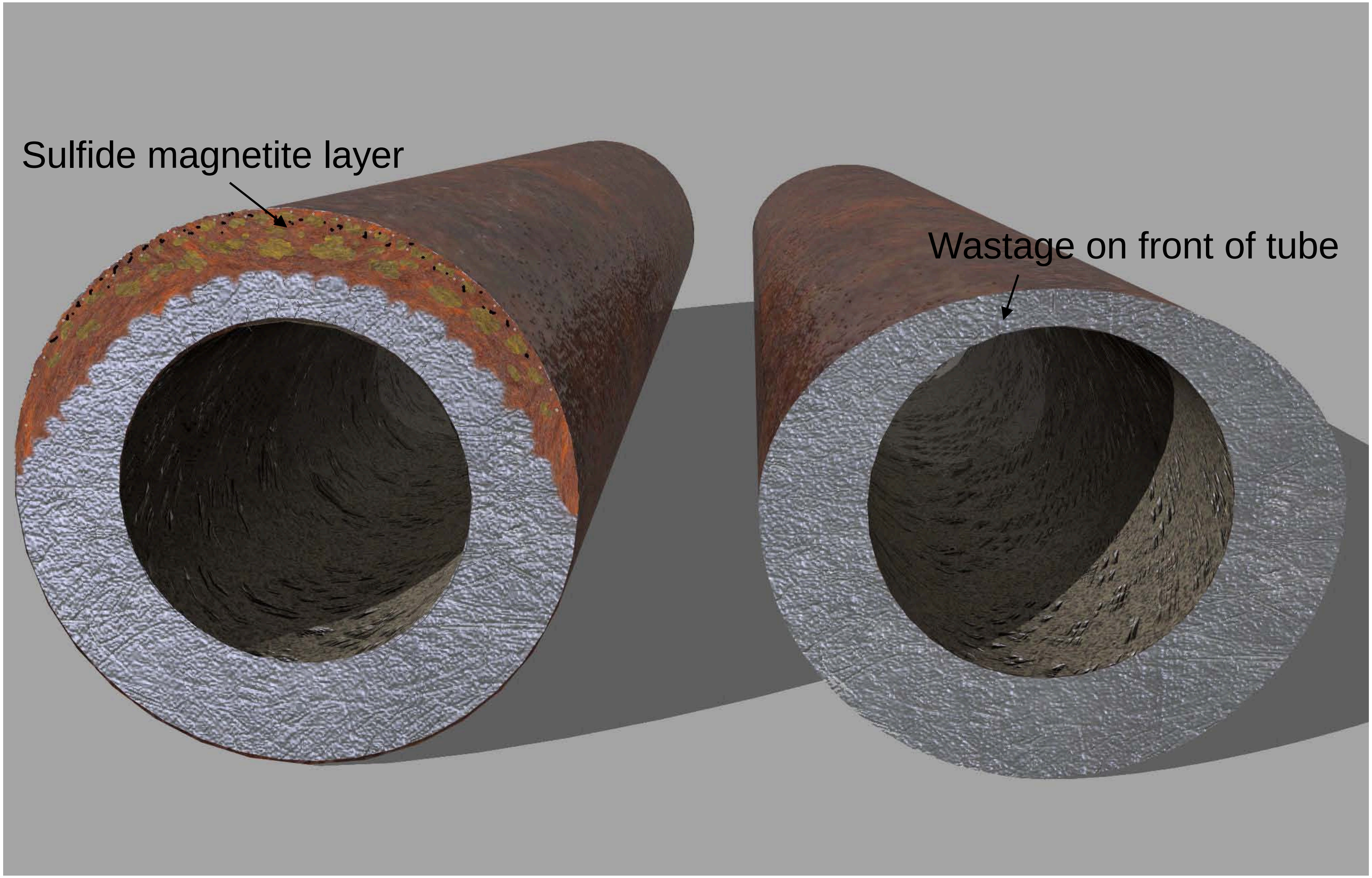


Image of simplifed coal fired power plant courtesy of http://en.wikipedia.org/wiki/Image:PowerStation2.svg

Fireside Corrosion of Waterwall Tubes



Objectives

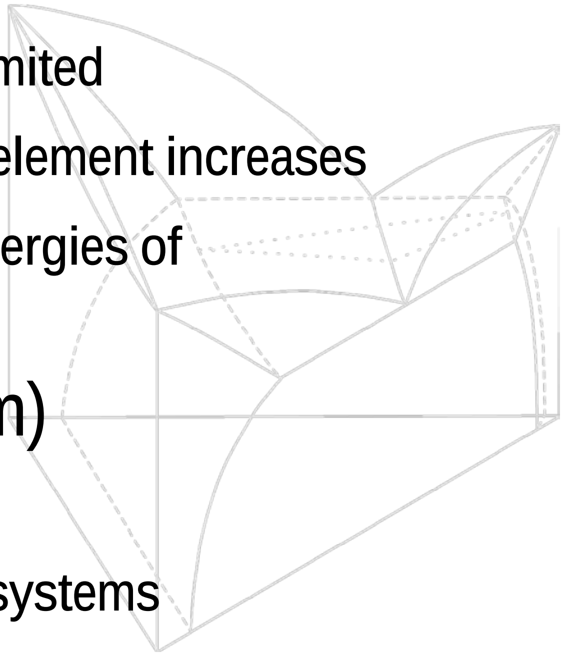
- FE-ARMP goals: “Develop a scientifically sound understanding of critical process issues confronting new coal-based energy systems, explore new avenues around critical crosscutting barriers, advance scientific knowledge across all coal and power systems”
- The development of TAILORED corrosion/sulfidation resistant surfaces based on scientific understanding from modeling/experiment
  - Work will initially focus on ferritic alloys (T22, nominal composition = 2.3 Cr, 0.1 Ni, 0.4 Mn, 0.3 Si, 1 Mo, 0.12 C, Fe bal)
    - Currently utilized tube metal selected as baseline substrate material
  - Initial experimental coatings will focus initially on existing protection compositions (aluminides) and potentially weld overlay compositions (Lehigh, etal…)
  - Will collaborate with other ARM projects (Pint, Santella , etal…) to maintain relevancy
- Key Issues
  - Thermal expansion
  - Thermal conductivity
  - Sulfidation/oxidation resistance
  - Metal surface properties (roughness, microstructure, chemistry, etc…)

Approach

- Thermo-chemical modeling
  - What is the perfect protective surface/compound?
  - Does it have the properties necessary to address key issues?
  - Can it be adapted to either be applied directly to tube outer wall or does a systems approach need to be utilized?
  - Results feed directly to experimental work
- Experimental Validation
  - Application of current protective systems using a low cost approach (surrogate material evaluation)
    - Evaluation of “state of the art” protective system on T22
  - Results feed directly to modeling work
  - Application, evaluation and testing of new candidate materials/surfaces
  - Characterization of metal surface properties (roughness, microstructure, chemistry, etc…) is vital to success of this task

Computational Thermodynamic Modeling

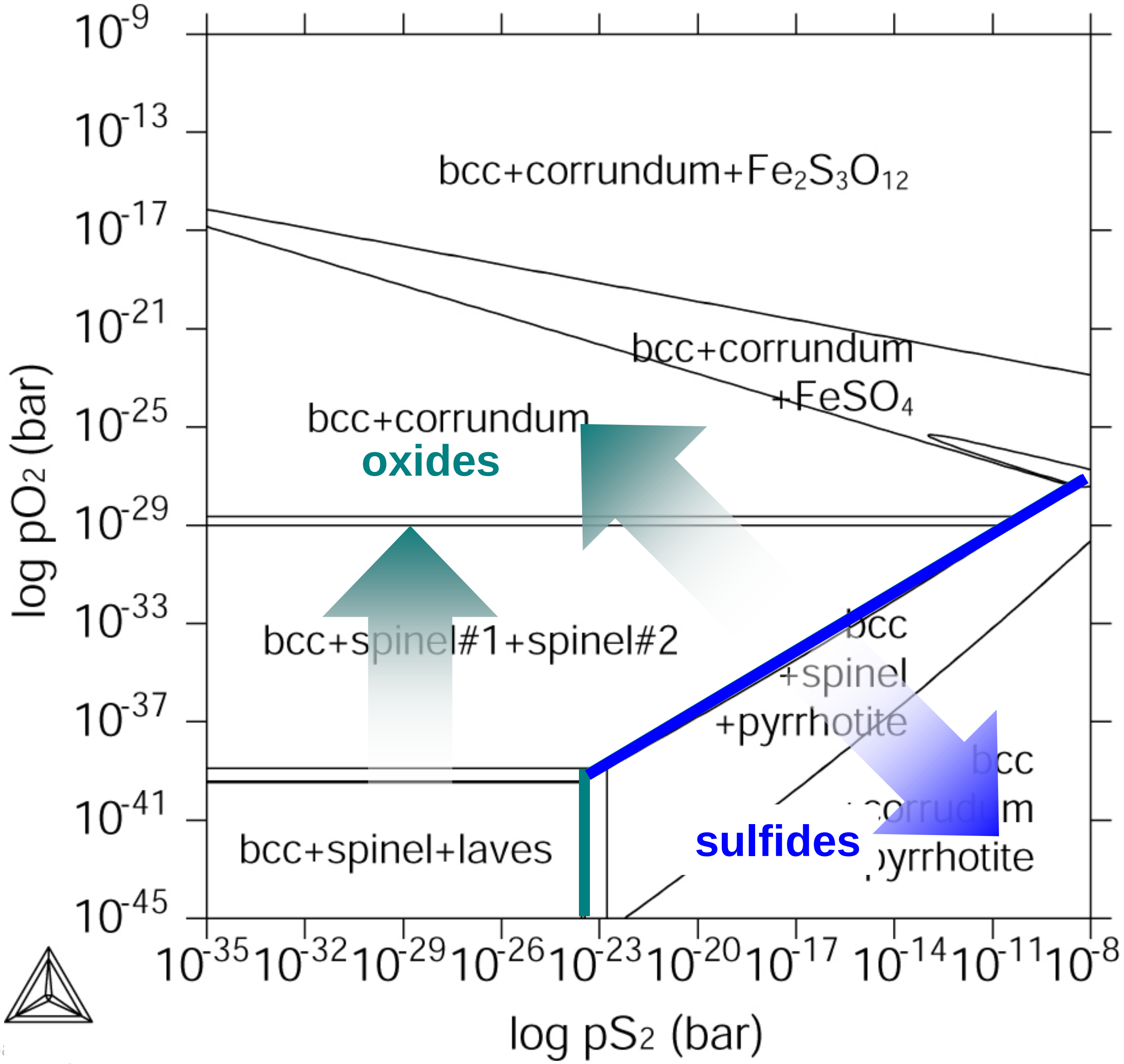
- Phase stabilities for fossil energy applications
  - Phases: ferrite, austenite, carbides, oxides, sulfides, …
  - Conditions: T, X, log P_{O_2}, log P_{S_2}, …
- Computational thermodynamics
  - T-X or T-P dimension that can experimentally visit is limited
  - Complexity increases exponentially as the number of element increases
  - Phase diagrams can be CALCULATED, when Gibbs energies of individual phases are available
- CALPHAD (CALculation of PHase Diagram) computational thermodynamic modeling
  - Evaluate Gibbs energies of phases in the lower order systems
  - Extrapolate to higher order system to predict phase stabilities at any give conditions (T, P, wt %, …)



Calculations Details

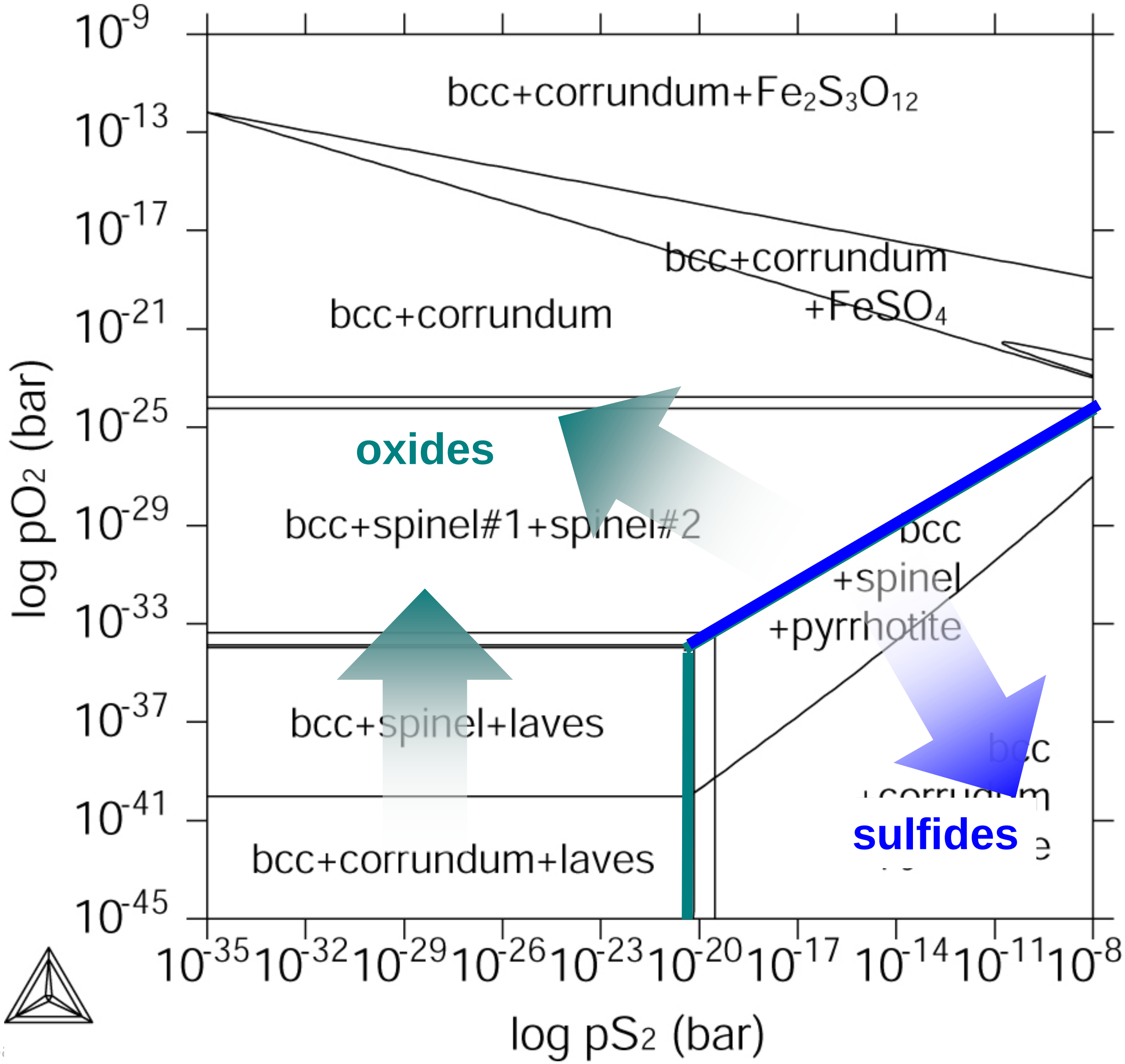
- TCFE6 Database
  - Fe with 21 elements
    - C, Al, Ar, B, Ca, Co, Cr, Cu, Mg, Mn, Mo, N, Nb, Ni, O, P, S, Si, Ti, V, and W
  - Self-consistent Gibbs energy functions for all the phases
- POLY-3 Gibbs energy minimizer in Thermo-Calc
- T22 nominal composition: Fe-2.25Cr-1Mo
- Oxygen and sulfur gas are considered for stability diagram
- Different temperatures: 400, 500 and 600C

Calculated Stability Diagram of T22 (400°C)



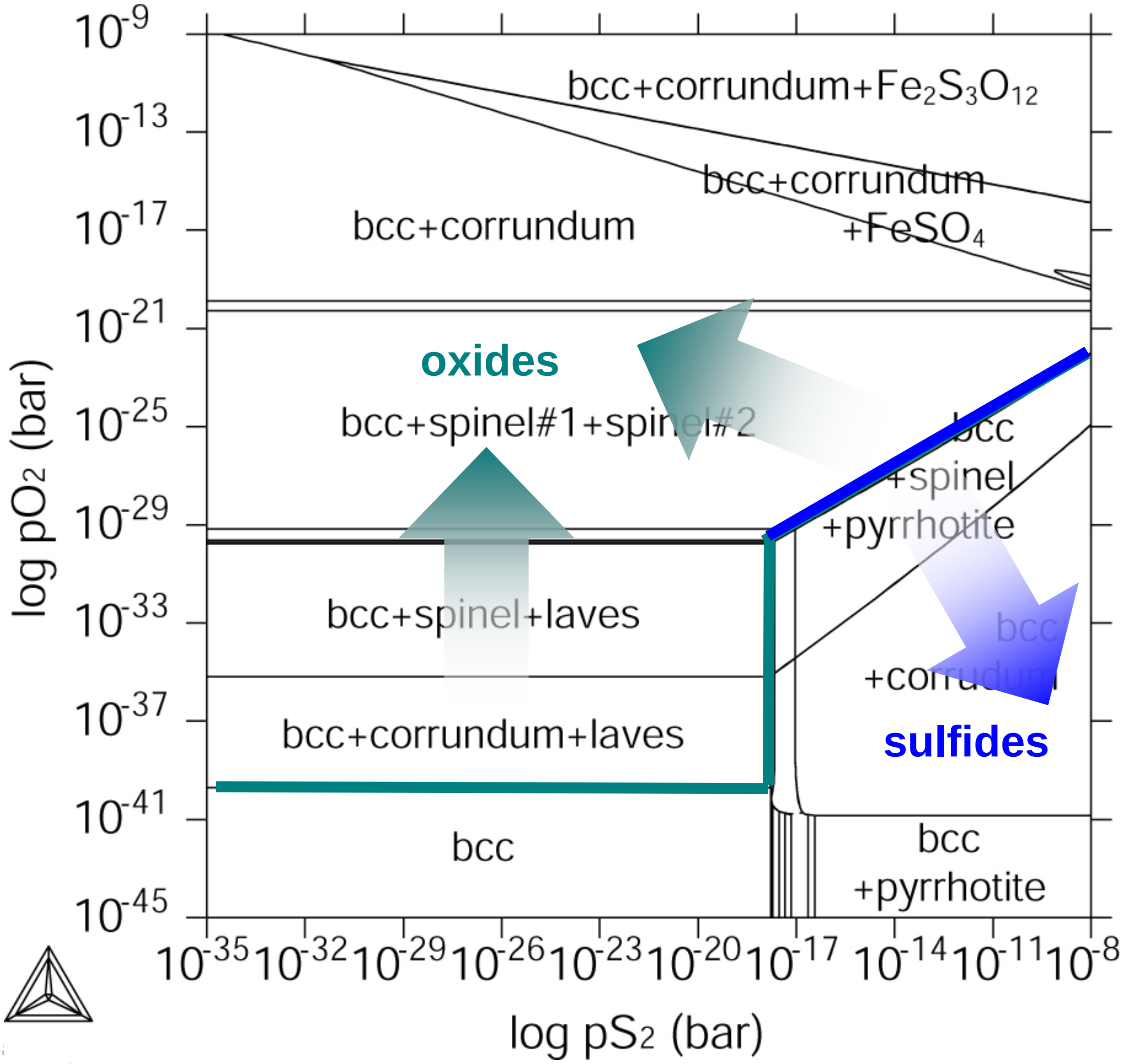
***Only Fe, Cr, Mo, O_2, S_2 are considered**

Calculated Stability Diagram of T22 (500°C)



***Only Fe, Cr, Mo, O_2, S_2 are considered**

Calculated Stability Diagram of T22 (600°C)



*Only Fe, Cr, Mo, O_2, S_2 are considered

Computational Modeling Approach

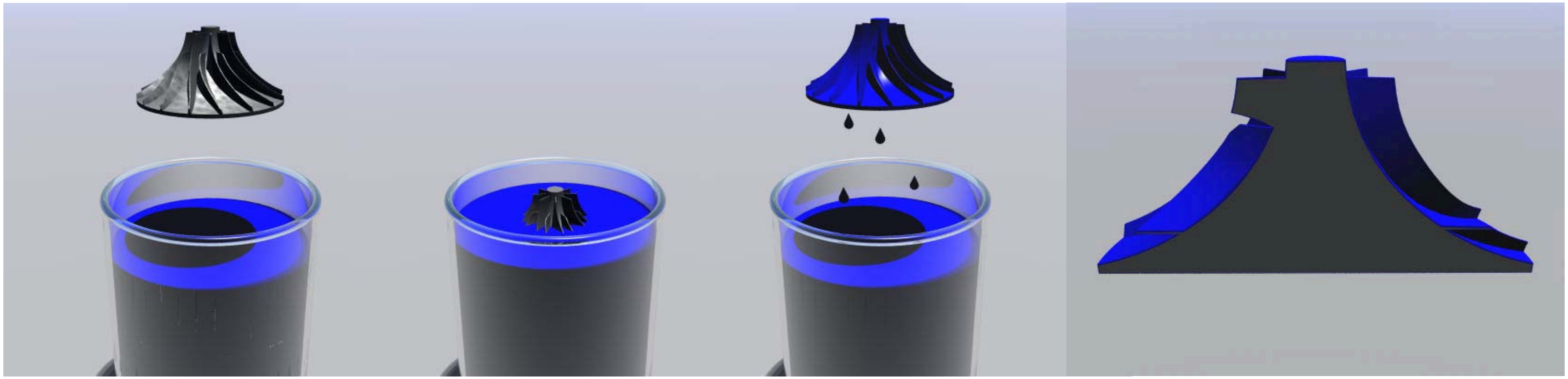
- Identifying materials thermochemically stable at working condition (T, X, log pO_2, log pS_2, …)
  - Literature search
  - Computational thermodynamic database search
- Predict the phase stability of coating materials with the presence of T22 and equilibrium gas composition
  - Computational screening to identify coating materials which are stable with T22 and equilibrium gas phase
- Perform experiments to validate predicted thermal stability of candidate coating materials

Experimental Validation

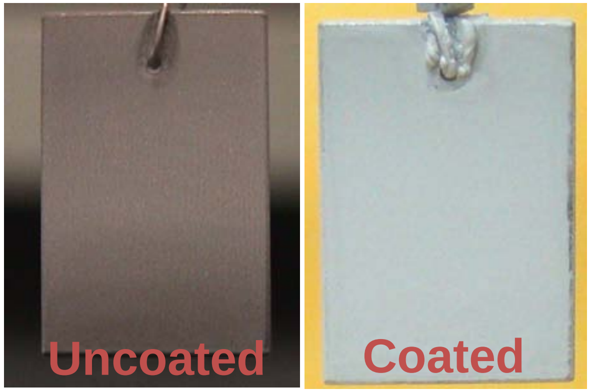
- Use existing “state of the art”
  - Aluminide coating
- Utilize ORNL’s slurry coating process to apply coatings
- Examine resulting microstructures
- Testing

What are Slurry Coatings?

- A slurry is metallic or ceramic mixture in which a material and a binder are suspended in a solvent

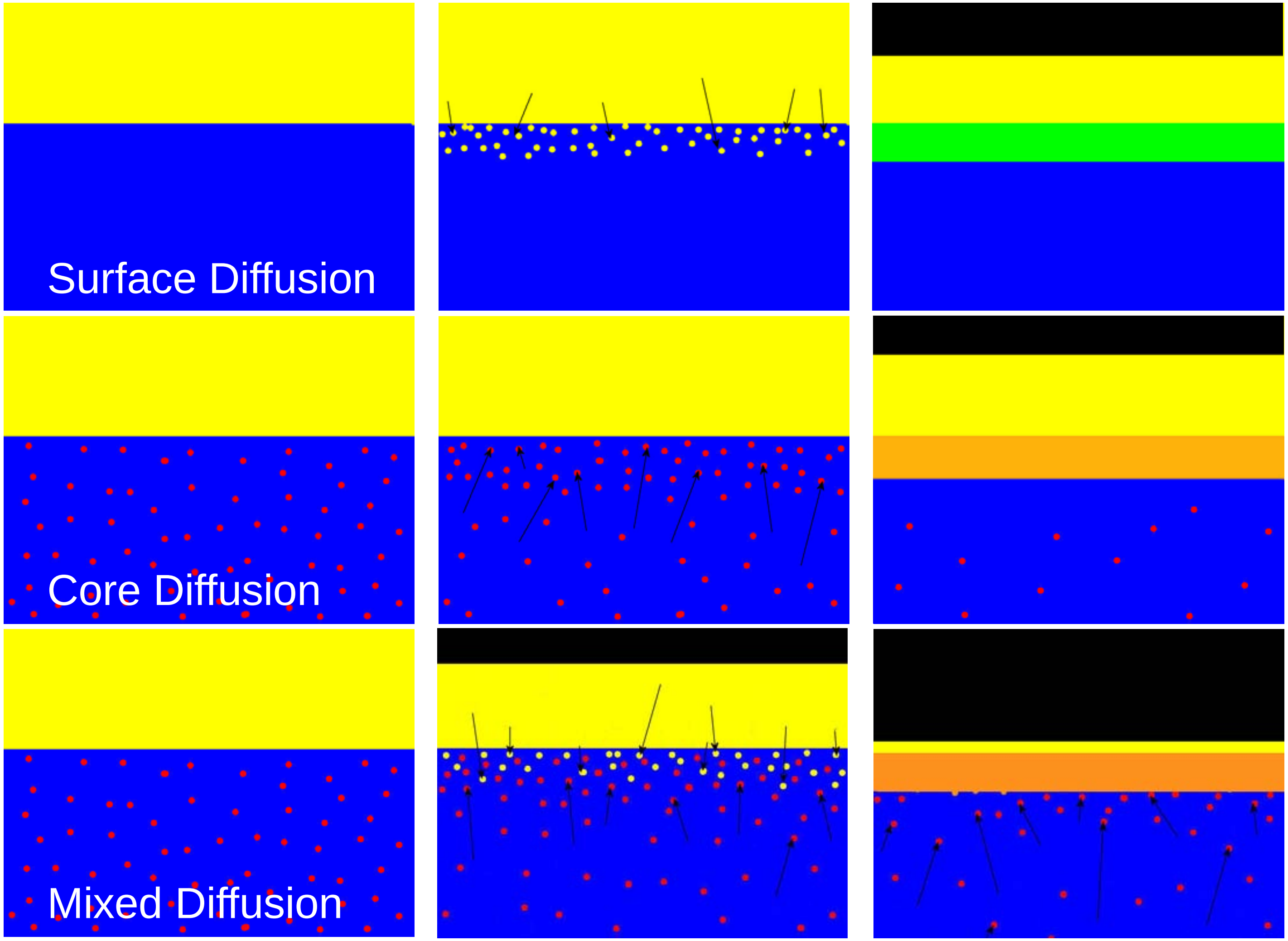


Benefits: Non-line-of-sight, can be used for complex shapes, no unique equipment needed, process can be automated

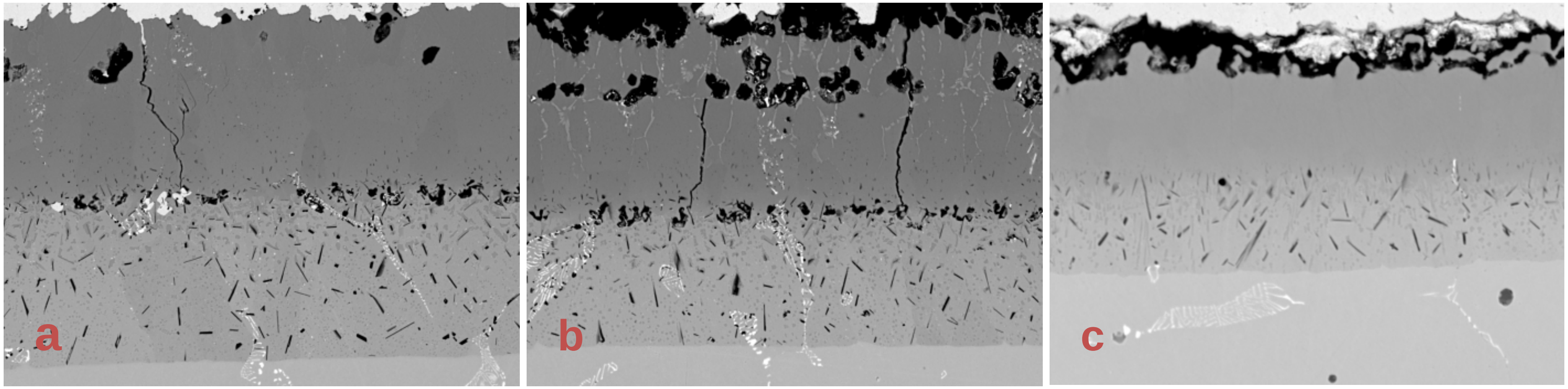


How Do Slurry Coatings Work?

- Heat treatment aids in the diffusion of “metal” into the substrate (leading to an enriched surface or formation of another phase)
- Once exposed to an environment, a protective scale can form

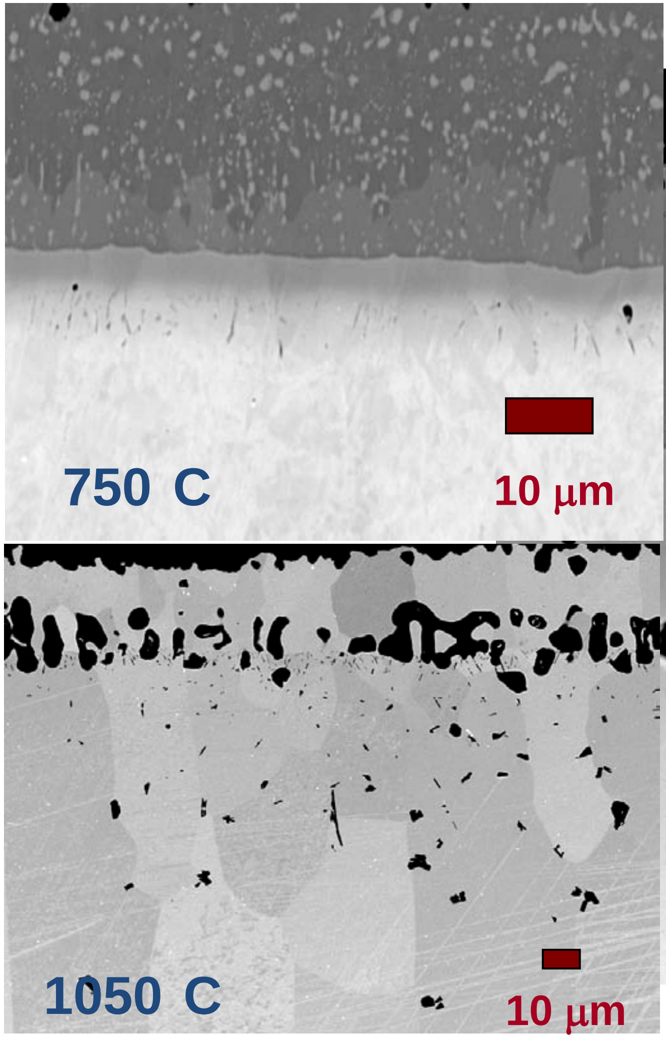


“The Devil is in the Details”



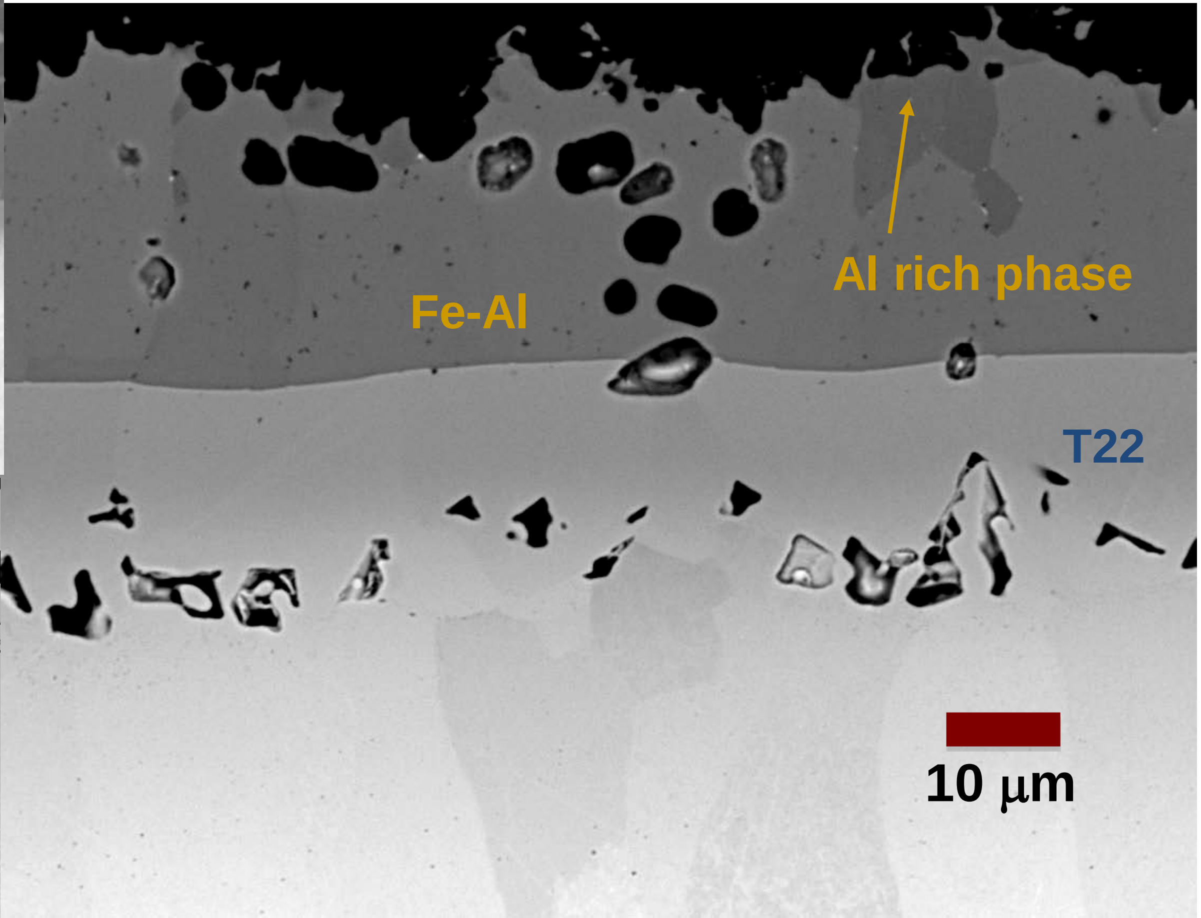
Back scattered electron images of as-fired aluminide slurry coatings on alloy CF8CP. (a) Commercial coating fired in vacuum at 1000°C, (b) commercial coating fired in Ar at 1000°C, (c) ORNL coating fired in Ar at 900°C.

Will the Real T22 Please Stand Up?



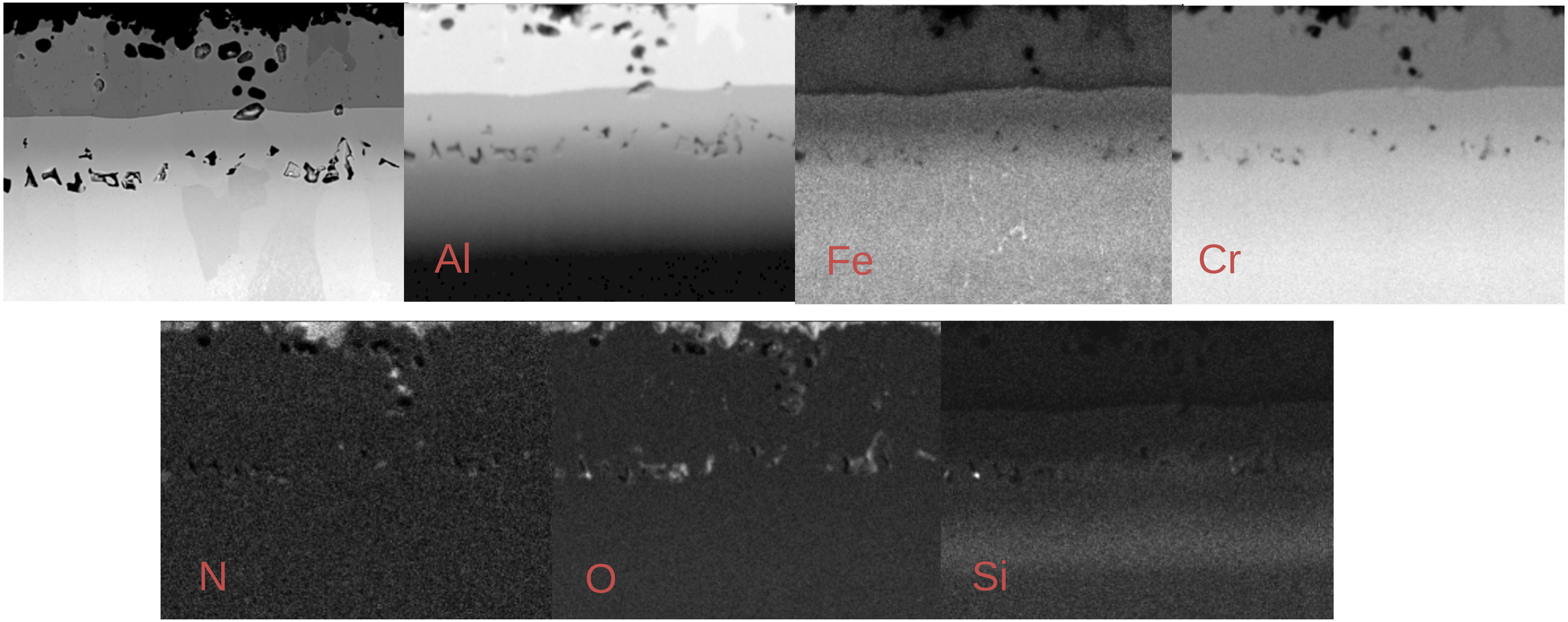
ORNL coating on P91
heat treated in Ar

ORNL coating on T22 fired in Ar at 900°C.



Composition and fabrication process (tube, plate, etc…) will affect coating/diffusion

Al Rich Phase Forming in Coating



Elemental solubility in alloy needs to be considered in modeling

Summary

- Thermochemical calculations initiated to determine baseline (equilibrium)
- Aluminum coatings applied to T22
  - Lower solubility of Al in ferritic structure seen at initial heat treatment temperature
- Milestones
  - Identify candidate material system for coating development and evaluation (5/30/10)
  - Complete characterization of substrate surface and colloid system (9/30/10)
  - Initiate coating deposition (9/30/10)
  - Complete testing of coated steels and apply Go/No-Go criteria (9/30/2011)
  - Using modeling approaches, determine if a graded-property approach is feasible, and identify coating thickness necessary (5/30/11)
  - Complete second iteration coatings based on results of FY2011 work (9/30/12)

Future Work

- Continue modeling
  - Begin adding alloying elements to equilibrium conditions
  - Begin non-equilibrium calculations for baseline
  - Computational screening for candidate materials
- Experimental
  - Complete evaluation of Al coating at alternative temperatures and heat treatment environments
- Testing

Acknowledgements

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Questions?

Reference Environments

Gas Composition in Furnace		
Vol %	Oxy-fuel fired PF	Air-fired PF
N_2	4.8	71.3
O_2	1.9	2.5
CO_2	58.9	15.3
H_2O	31.8	10.0
Ar	2.1	0.8
SO_2	0.49	0.13

B. Bordenet and F. Kluger, *Mater. Sci. Forum,* ***595-598*** *(2008) pp 261-269*