# Computational Design of Crack-Resistant W-Nb-C Alloy for LPBF

Analysis Based on "Near crack free additive manufacturing of a novel W-Nb-C alloy"

# Overview

# Q1: Thermodynamic Strategy for Crack Resistance

## Primary Objective

Maintain "crack-healing" mechanism in W-15Nb-C alloy through controlled eutectic solidification

## Key Challenge

Ensure liquid phase availability during critical solidification stages to prevent hot tearing and enable crack backfilling

# Governing Thermodynamic Parameters (Part 1)

## 1. Solid Fraction at Eutectic Onset ($F_{s,eutectic}$)

- **Role:** Timing of crack-healing liquid availability
- **Target:** $F_{s,eutectic} > 0.65$
- **Effect:** Liquid must appear AFTER stress development

## 2. Dendritic Coherency Point ($F_{s,DCP}$)

- **Role:** Stress initiation point
- **Critical Condition:** $F_{s,eutectic} > F_{s,DCP}$
- **Effect:** Liquid reservoir remains after stress buildup

# Governing Thermodynamic Parameters (Part 2)

## 3. Eutectic Temperature Range ($\Delta T_{eutectic}$)

- **Role:** Duration of healing process
- **Target:** Wide temperature plateau
- **Effect:** Prolonged stress relaxation window

## 4. Terminal Solidification Slope ($dT/df_s$)

- **Role:** Final-stage healing effectiveness
- **Target:** Shallow slope near $F_s = 1$
- **Effect:** Maximum time for liquid backfilling

# Optimization Strategy Summary

## Target Solidification Profile

1. **Rapid initial solidification** to form dendritic skeleton
2. **Late eutectic onset** ($F_s \sim 0.7$) after coherency
3. **Wide, flat eutectic plateau** for prolonged healing
4. **Shallow terminal slope** for final crack sealing

## Success Criteria for W-15Nb-C

Scheil simulation must show eutectic reaction beginning after dendritic coherency and persisting with minimal temperature change until complete solidification

# Q2: Computational Workflow Overview

## Primary Objective

Quantify oxygen segregation tendency and embrittlement effect at critical interfaces using first-principles methods

## Target Interfaces

1. W-rich SS / NbC interphase boundary
2. W-rich SS grain boundaries

## Primary Method

Density Functional Theory (DFT)

- Software: VASP
- Pseudopotentials: PAW
- Functional: PBE

# Three-Step DFT Workflow

## Step 1: Interface Structure Modeling

- Construct atomic supercells of target interfaces
- Find most stable configurations via energy minimization
- Model both coherent and semi-coherent interfaces

## Step 2: Oxygen Segregation Energy

$$E_{seg} = E_{\text{interface+O}} - E_{\text{interface}} - \mu_O$$

- Negative value indicates favorable segregation
- Compare multiple interface sites
- Reference $\mu_O$ to $O_2$ molecule or bulk W

## Step 3: Work of Separation

$$\gamma_{sep} = \frac{E_{\text{slab1}} + E_{\text{slab2}} - E_{\text{interface}}}{2 \times \text{Area}}$$

- Quantifies interfacial cohesion strength
- Compare $\gamma_{sep}^{\text{clean}}$ vs $\gamma_{sep}^{\text{with O}}$
- Large reduction indicates severe embrittlement

# Validation & Databases

## Computational Resources

- **VASP** with PAW pseudopotentials
- **Materials Project** database
- **NIST** reference data for benchmarking

## Validation Methods

- **XPS:** Core-level binding energy shifts
- **STEM-EELS:** Direct interface chemistry
- **SEM Fractography:** Fracture path analysis

## Predicted Correlation

Strong oxygen segregation at W/NbC interface + reduced $\gamma_{sep} \rightarrow$ SEM shows interphase fracture along segregation channels

# Q3: Multi-scale Modeling Approach

## LPBF Challenge

Extreme cooling rates ($10^5$-$10^7$ K/s) cause:

- Severe microsegregation
- Solute trapping
- Metastable phase formation
- Retained supersaturation

## Standard CALPHAD Limitation

Equilibrium assumptions invalid under LPBF conditions - requires kinetic coupling

# Hierarchical Computational Framework

## 1. DICTRA Simulations

**Inputs:**

- CALPHAD thermodynamic database
- Mobility database
- Initial composition
- Cooling rate ($10^6$ K/s)

**Outputs:**

- Phase fractions vs. time
- Composition profiles
- Solute trapping extent

## 2. Phase-Field Modeling

**Coupled with CALPHAD:**

- Dendritic morphology
- Eutectic structure
- Metastable phases

**Output:** Microstructure evolution

## 3. Advanced Scheil Model

- Clyne-Kurz back-diffusion
- Quick microsegregation estimate
- Screening tool

# Heat-Treatment Design Guidance

## Homogenization Treatment

**Using DICTRA:**

- Input: Microsegregation profiles from LPBF simulation
- Simulate annealing (1200-1400°C)
- Optimize time to achieve homogeneity
- Prevent excessive grain growth

## Precipitation Hardening

**Using CALPHAD:**

- Calculate TTT/CCT diagrams
- Identify solvus temperatures
- Design aging treatments
- Control carbide precipitation

## Integrated Workflow

LPBF Process $\rightarrow$ Non-equilibrium Simulation $\rightarrow$ Optimized Heat Treatment $\rightarrow$ Enhanced Properties

# Integrated Computational Materials Engineering

## Multi-scale Approach Success

- **CALPHAD:** Thermodynamic-guided alloy design
- **DFT:** Fundamental interface properties
- **DICTRA/Phase-Field:** Process simulation
- **Complementary methods** for comprehensive understanding

## Impact on Additive Manufacturing

This framework enables **rational design** of crack-resistant refractory alloys, significantly reducing trial-and-error experimentation and accelerating development of high-performance materials for extreme environments.

# Thank You