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 μ_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

Questions