Advanced Materials for the Lunar Surface: Multiscale Computational Design of Refractory Alloys and Carbides

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ANALYTICAL MECHANICS ASSOCIATES

Background

High-fidelity computational modeling provides a safe, cost-effective alternative to hazardous high-temperature testing. This poster highlights simulation-driven materials development for two critical applications: nuclear propulsion propellant channel coatings and refractory alloy additive manufacturing.

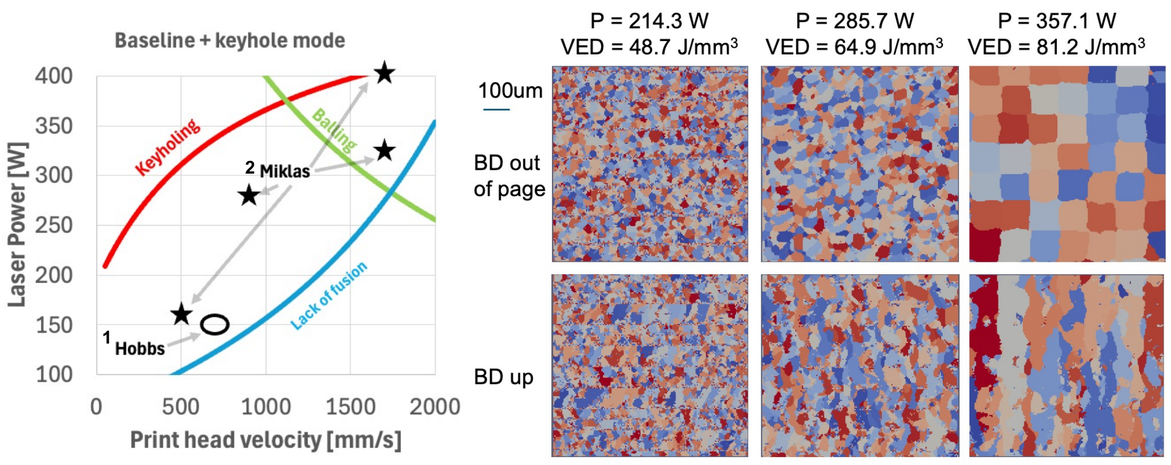
Multiscale Modeling for AM Alloy Design, Optimization, and discovery[3]

AM Optimization Framework: A predictive toolset mapping process-structure-property relationships for AM alloys.

Melt-Pool Physics: Validated multiscale models to predict optimal processing parameters (Inconel 625, C-103).

Microstructure Prediction: Validated Kinetic Monte Carlo models simulating LPBF build structures (316L, Inconel 625, C-103).

Mechanical Response: Linked molecular dynamics, dislocation dynamics, and crystal plasticity FEM to model alloy hardening mechanisms.



Note: as-printed microstructures; constant print velocity V = 1000 mm/s

Predicted C103 printability map and printed microstructures

Alloy discovery

Objective: Develop economical, printable C-103 replacements (Yield Strength > 250 MPa at 1300 C; Density < 9.0–10.2 g/cm³).

Methodology: Leveraged multiscale modeling for rapid screening of the **Nb-W-Mo-Zr** composition space.

Optimization: Substituted costly Hf with **Zr** for oxidation resistance, using computational design to successfully maintain AM printability.

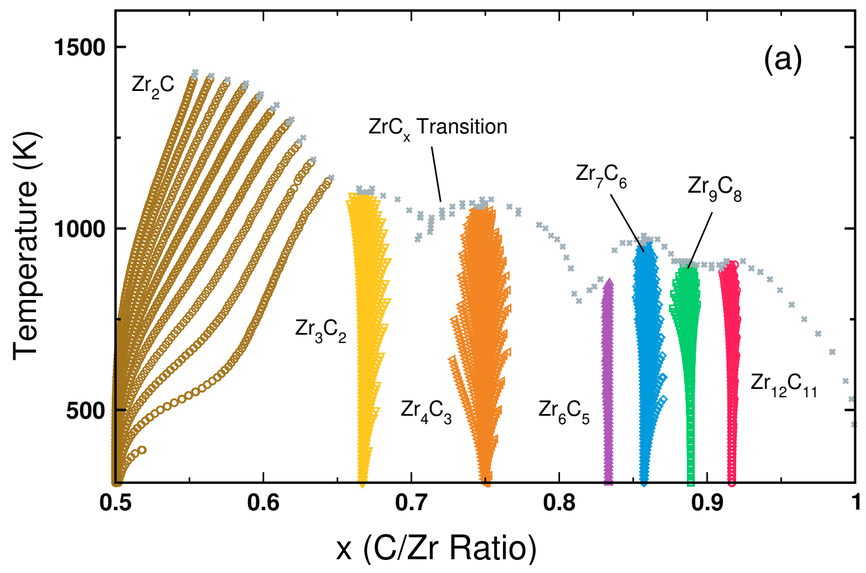
Predicted properties outperform C103

Alloy (Density)	Hot cracking	Strength at 1300 C	S-L range
C103: Nb-10Hf-1Ti	1.1	95 MPa	336 K
Nb-ARC1 (9 g/cm³)	0.6	> 3x C103	< C103
Nb-ARC2 (10.2 g/cm³)	0.8	5x C103	< C103
Nb-ARC3 (9 g/cm³)	0.7	> 5x C103	< C103
Nb-ARC4 (10.2 g/cm³)	0.8	6x C103	< C103

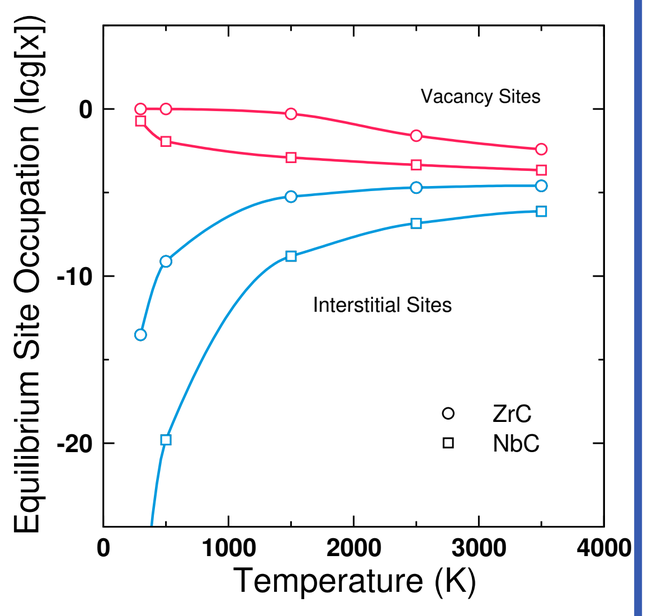
Carbides for nuclear propulsion[4]

Thermodynamic databases built from highly accurate first principles methods yield predictive phase diagrams and reaction equilibria that allow engineering-scale relevance

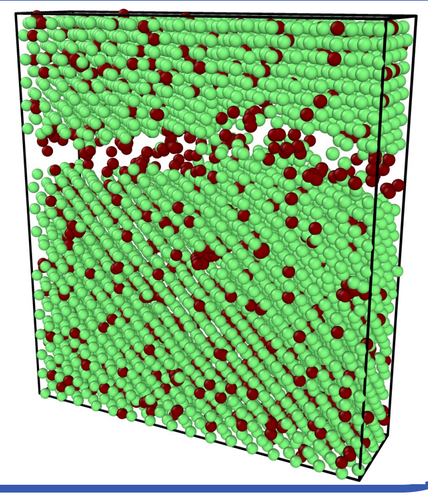
Material stability: Three new vacancy-ordered phases of ZrC predicted: Zr_6C_5 (P1), Zr_9C_8 (R3), and $Zr_{12}C_{11}$ (C2/m)



Hydrogen and vacancy interactions: Reaction databases utilized to predict the performance tradeoffs of various propellant channel coatings[5]



Fracture toughness: Highly accurate interatomic force fields, trained from first principles data, can be used to study atomic-scale fracture of these carbides when hydrogen is present



Potential collaboration areas

- Fission Surface Power:
  Alloy processing/properties for hot structures
- Nuclear Propulsion
  - Propellant channel coating development
- In-Situ Resource Utilization
  - Regolith sintering & processing for infrastructure
- Dust mitigation
  - Coating material development and discovery

Modeling expertise: Material Response, Gas Surface Interactions, Microscale / Mesoscale, Atomistic (MD) / Ab Initio (DFT) , CALPHAD, Thermo-Structural, Machine Learning

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REFERENCES: [1]Private communication with Toren Hobbs. [2]Miklas, A. Additive Manufacturing of Refractory Alloys. M.Sc. thesis, Colorado School of Mines, 2022. [3]W C Tucker, J Cho, K Doss, K Wheeler, and L J Abbott. A multiscale predictive framework for process and property modeling of refractory additively manufactured alloys. Technical report, in prep, NASA Ames Research Center, Mountain View, CA, 2026. [4]J B Haskins, J Cho, W C Tucker, L J Abbott, and G Costa. Computational Thermodynamics of Ordered and Disordered ZrC Vacancy Structures. Physical Review B, in review, 2026. [5]W C Tucker, J Cho, and J Haskins. Characterizing the carbon depletion and hydrogen enrichment of ZrC and NbC in high-temperature hydrogen via ab initio simulation. Journal of Nuclear Materials, in review, 2026.

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