

# Enabling Solar Thermal Propulsion with Computational Materials Design



Justin Haskins,<sup>1</sup> Lauren Abbott,<sup>2</sup> Piyas Chowdhury,<sup>2</sup> William Tucker,<sup>2</sup> Charles Bauschlicher,<sup>1</sup> Donald Ellerby<sup>3</sup>

<sup>1</sup>Thermal Protection Materials Branch, NASA Ames Research Center

<sup>2</sup>AMA, Inc., Thermal Protection Materials Branch, NASA Ames Research Center

<sup>3</sup>Entry Systems and Vehicles Development Branch, NASA Ames Research Center

## 1. Background and Challenge

**Solar thermal propulsion (STP) promises high specific impulse** (1200 s) for missions to the interstellar medium (5x faster than Voyager):

- H<sub>2</sub> propellant heated up to 3500 K during close Solar approach
- Heat exchanger (HX) must survive 5 hours in hot H<sub>2</sub>
- Baseline uses refractory coatings to protect a carbon/carbon HX

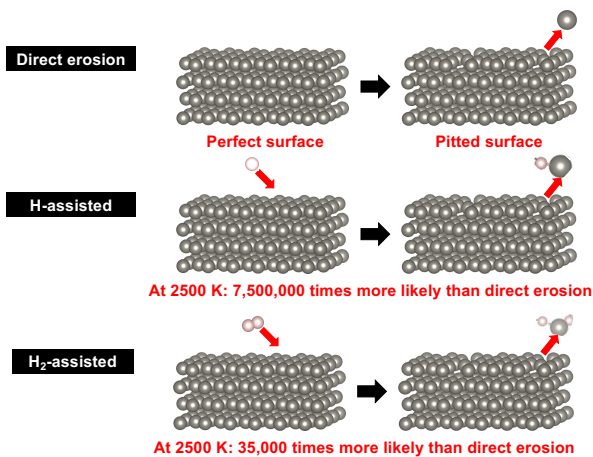
## 2. Key Objectives

Use **multiscale computational techniques** to **inform coating material and design** by characterizing:

- Surface reactions and erosion
- Mechanical response and fracture during operation
- Integrated material response during operation

## 3. Coating Surface Reaction

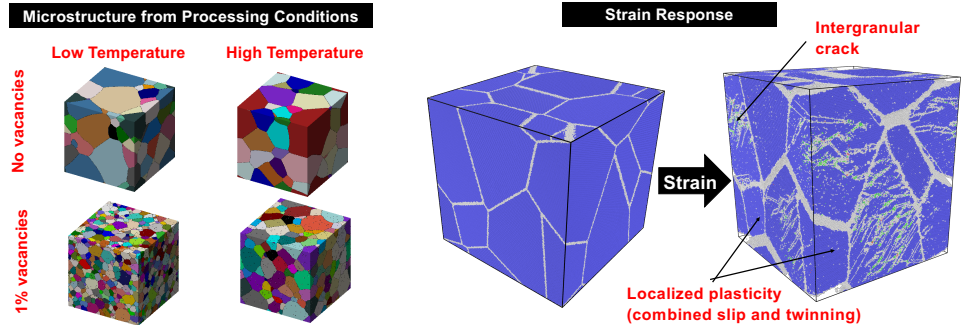
Tungsten Case Study: Erosion occurs through surface reactions with hydrogen propellant.



Methods include thermodynamics from quantum simulations.

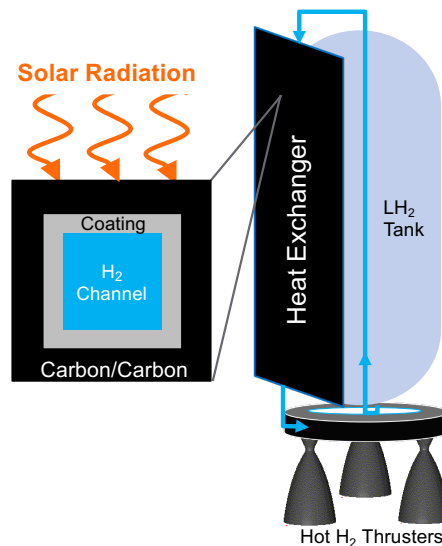
## 4. Coating Mechanical Response and Fracture

Tungsten Case Study: Grains govern balance between plastic deformation and cracking.



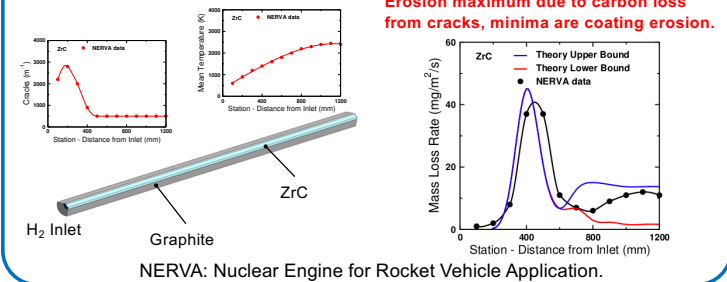
Methods include molecular dynamics, Monte Carlo, and discrete dislocation dynamics simulations.

## Solar Thermal Propulsion



## 5. Comparison with Heritage Operational Data

NERVA Case Study: Model observed mid-range corrosion of ZrC in hot H<sub>2</sub> channels to understand origins.



## 6. Engagement and Forward Work

Engaged with development efforts for:

- **STP** coating material selection with **JPL**
  - **Nuclear thermal propulsion** coatings and fuel materials material response with **MSFC**
- Future work: Predictive modeling of fracture/crack density