Enabling Solar Thermal Propulsion with Computational Materials Design

Justin Haskins,1 Lauren Abbott,2 Piyas Chowdhury,2 William Tucker,2 Charles Bauschlicher,1 Donald Ellerby3

1Thermal Protection Materials Branch, NASA Ames Research Center  
2AMA, Inc., Thermal Protection Materials Branch, NASA Ames Research Center  
3Entry 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):
- H₂ propellant heated up to 3500 K during close Solar approach  
- Heat exchanger (HX) must survive 5 hours in hot H₂  
- 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.

Direct erosion
- Perfect surface  
- At 2500 K: 7,500,000 times more likely than direct erosion

H-assisted
- Pitted surface  
- At 2500 K: 35,000 times more likely than direct erosion

H₂-assisted
- Erosion maximum due to carbon loss from cracks, minima are coating erosion.

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.

5. Comparison with Heritage Operational Data
NERVA Case Study: Model observed mid-range corrosion of ZrC in hot H₂ channels to understand origins.

NERVA: Nuclear Engine for Rocket Vehicle Application.

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