Computational Materials Techniques for Thermal Protection Solutions: Materials and Process Design

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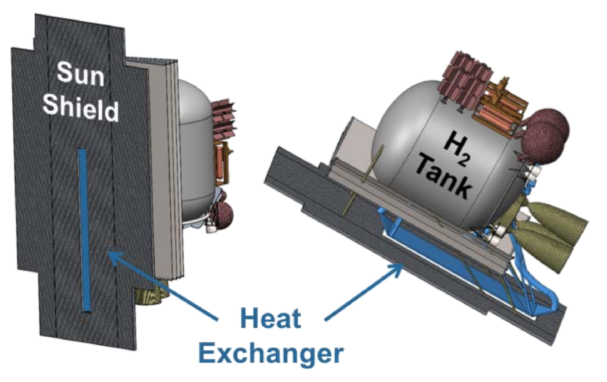
Example 1: Materials Design for Solar Thermal Propulsion[a]

Problem

Solar thermal propulsion (STP) is a leading candidate for high-velocity travel into the interstellar medium (enables 15 AU/year compared to Voyager's speed of 3.6 AU/year). STP requires a close approach to the sun (3-4 solar radii) to heat a hydrogen (H_2) fuel to 3100-3500 K, which will then be ejected through a nozzle for thrust.

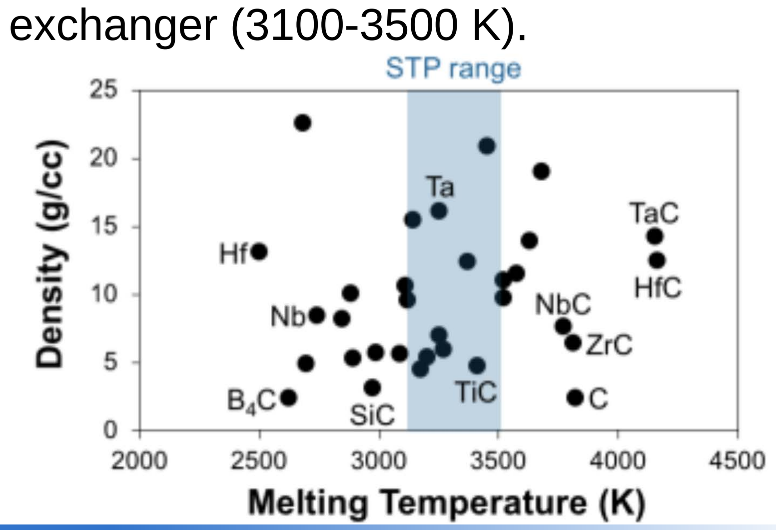
STP requires a heat exchanger material to transfer solar radiation to the fuel. The leading candidate is a coated carbon/carbon material. The goal is to computationally screen for a coating material that does not melt, is chemically inert to a H_2 fuel, a diffusive barrier to H_2 fuel, and sized to prevent ablation from vaporization.



Results and Discussion

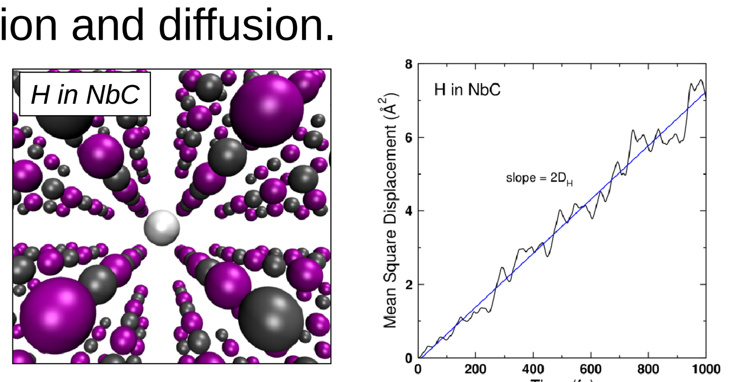
Melting Point

The melting points of coating candidates must be higher than the operation temperature of the STP heat exchanger (3100-3500 K).



Diffusion

Hydrogen atoms can adsorb onto the coating surface and diffuse through the material, embrittling the material or reacting with carbon. *Ab initio* molecular dynamics is used to characterize adsorption and diffusion.



Adsorption is not favored and H_2 prefers to remain in the gas phase at STP conditions. For H_2 that does adsorb, diffusivity is high (~15 mm/hr).

Reactions

Reactions with hydrogen occur that can degrade the surface or lead to the evolution of gaseous products. These are characterized using quantum thermochemistry.

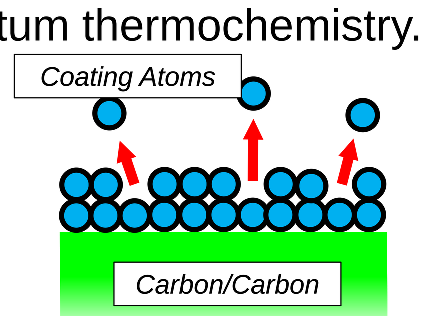
Coating Material Reaction	ΔG
$HfC(s) + 3H_2(g) \rightarrow HfH_2(s) + CH_4$	6.3
$2TaC(s) + 5H_2(g) \rightarrow TaH_2(s) + 2CH_4(g)$	7.5
$NbC(s) + 3H_2(g) \rightarrow NbH_2(s) + CH_4(g)$	6.2
$W(s) + 2H_2(g) \rightarrow WH_4(g)$	2.0
$2Re(s) + 3H_2(g) \rightarrow 2ReH_3(g)$	4.2

Reaction free energies of coating materials with hydrogen at the operation temperatures of STP are positive, meaning reaction is not favored. Loss H_2 of high entropy during reaction drives stability.

Ablation

Ablation is caused by the vaporization of coating atoms that enter the fuel flow and are removed. This is characterized by equilibrium vapor pressures obtained from quantum thermochemistry.

At conditions for STP (3500 K; 50 psi; 5 hrs), the coatings ablate by 1-3 mm. Carbides exhibit less ablation than refractory metals.



To summarize, coating materials have been computationally screened for suitability in a heat exchanger for solar thermal propulsion. Overall, high-temperature carbides are found to react minimally, prevent significant hydrogen intercalation and diffusion, and ablate by 1-3 mm during operation and represent the most promising candidates.

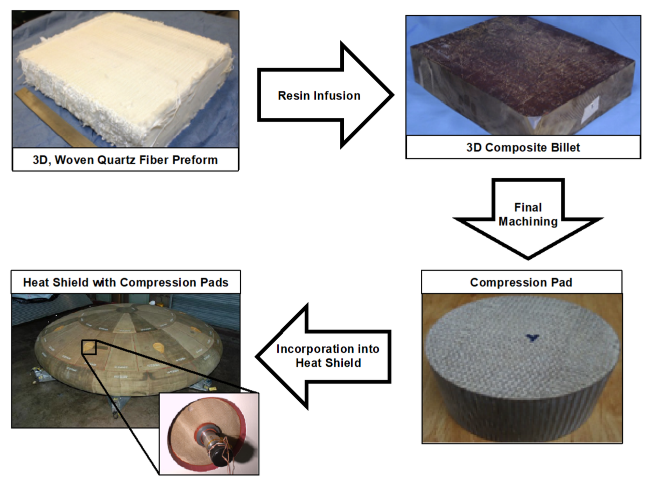
[a]Collaboration with: Don Ellerby (NASA), Dean Cheikh (Jet Propulsion Laboratory)

Example 2: Process Design for Heat Shield Composites[b]

Problem

The 3-Dimensional Multi-functional Ablative Thermal Protection System (3DMAT) is a fused quartz / cyanate ester composite used as the compression pad on the Orion EM-1 vehicle. This effort set out to produce fully densified 3-D orthogonally woven composite with less than 2% porosity.

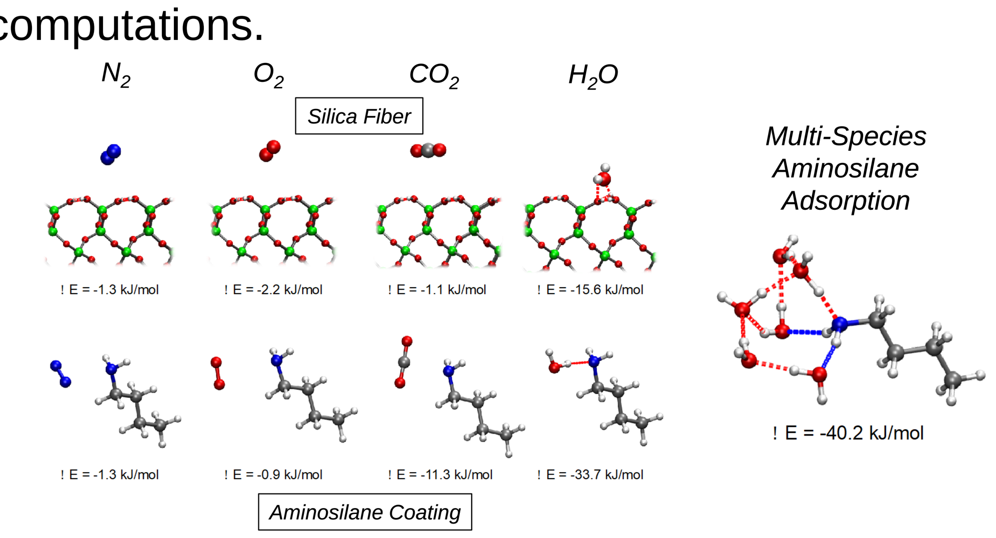
After infusing and the fused quartz preform with cyanate ester and curing, a large void has been observed in the center of some material samples. The void more frequently appears in large sized samples. Computational techniques are used to examine potential sources of the void, which include trapped residual gases and resin shrinkage during the cyanate ester cure phase.



Results and Discussion

Gas Adsorption

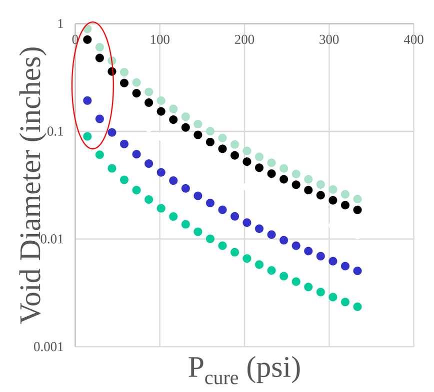
Gas adsorption on the preform and coating can lead to gas trapping and void formation during resin infusion. Water is found to be strongly adsorbed on the aminosilane coating from quantum chemistry computations.



Void Sizes

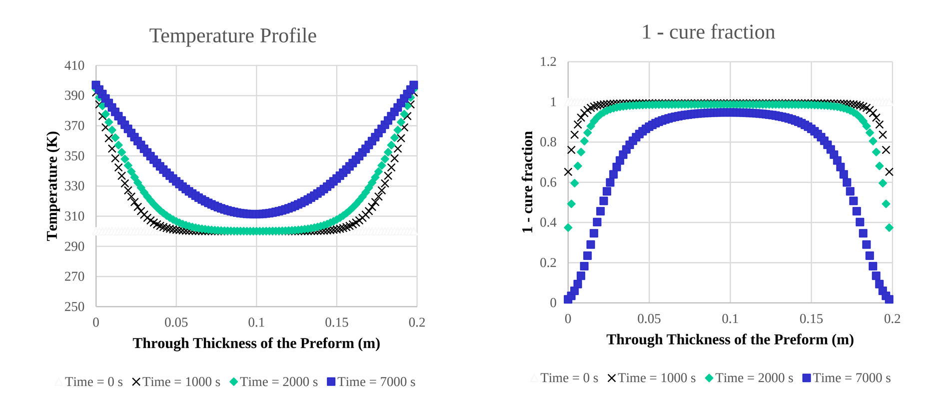
Gas adsorption and cure shrinkage cooperatively act to establish voids in the center of large billets. The size of the void is estimated from the quantity of adsorbed gas and cure dynamics.

For samples of 13"x12"x3" the interior pressure at the cure temperature of 310 ºF is reduced by these effects and voids of diameters of roughly half an inch are expected, in agreement with observation.



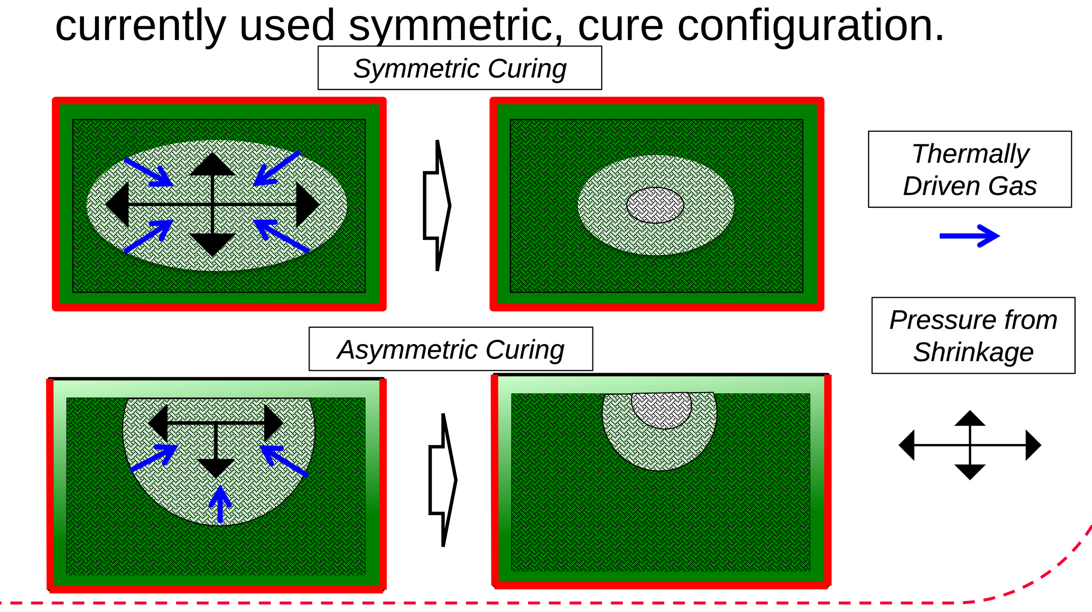
Cure Shrinkage

Cure dynamics using finite element modeling are performed for a hypothetical cyanate ester resin. During cure, the edges of the billet harden first, and subsequent curing and cure shrinkage leads to a pressure reduction from 100 psi to near ambient conditions at the center of the material.



Process Modification

One process modification to prevent void formation would be to adopt an asymmetric, versus the currently used symmetric, cure configuration.



To summarize, a computational process design study has been performed on resin infusion and cure for the 3-Dimensional Multi-functional Ablative Thermal Protection System to prevent the formation of voids. The results indicate moisture adsorption and resin shrinkage can lead to void formation in a symmetric curing configuration. An asymmetric curing configuration would not promote the formation of central voids.

[b]Collaboration with: Jay Feldman (NASA), Peter Gage (Neerim Corp.)