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

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Integrated computational materials techniques that span the atomistic and continuum scales have the potential to aid the design and manufacturing of thermal protection materials. Two cases demonstrating the practical application of these methods are discussed. Case one examines the selection of a high temperature coating for carbon/carbon, with the target application being a solar thermal propulsion heat exchanger. The performance of various refractory metal and metal-carbide coatings is characterized considering extreme thermal (3500 K) and chemical (hydrogen flows) conditions. The recession rate, hydrogen leakage, and likelihood of mechanical failure are characterized and provide directions for further experimental investigation. Case two examines the process optimization of a heat shield material composed of a woven silica fiber preform and cyanate ester resin. Frequently, internal voids were found to be present in this composite after the resin infusion and curing stages of manufacturing. Using the manufacturing conditions, computations indicate that both water adsorption and resin cure shrinkage are contributing factors to void formation. The results suggest an alternative process configuration for curing that would mitigate voids.