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Multiscale Process Modeling of Ceramic Matrix Composites

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Abstract : Ceramic matrix composites (CMCs) are typically used in applications that require long-term mechanical integrity at elevated temperatures. CMCs are usually fabricated using a polymer precursor that is initially polymerized in situ with fiber reinforcement, followed by a series of cycles of pyrolysis to transform the polymer matrix into a rigid glass or ceramic. The pyrolysis step typically generates volatile gasses, which creates porosity within the polymer matrix phase of the composite. Subsequent cycles of monomer infusion, polymerization, and pyrolysis are often used to reduce the porosity and thus increase the durability of the composite. Because of the significant expense of such iterative processing cycles, new generations of CMCs with improved durability and manufacturability are difficult and expensive to develop using standard Edisonian approaches. The goal of this research is to develop a computational process-modeling-based approach that can be used to design the next generation of CMC materials with optimized material and processing parameters for maximum strength and efficient manufacturing. The process modeling incorporates computational modeling tools, including molecular dynamics (MD), to simulate the material at multiple length scales. Results from MD simulation are used to inform the continuum-level models to link molecular-level characteristics (material structure, temperature) to bulk-level performance (strength, residual stresses). Processing parameters are optimized such that process-induced residual stresses are minimized and laminate strength is maximized. The multiscale process modeling method developed with this research can play a key role in the development of future CMCs for high-temperature and high-strength applications. By combining multiscale computational tools and process modeling, new manufacturing parameters can be established for optimal fabrication and performance of CMCs for a wide range of applications.

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