MULTIPHYSICS-MULTISCALE MODELING OF SEVERE-ENVIRONMENT MATERIALS

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Demands on materials performance in the severe high heat-flux environment of space and energy technologies necessitate a new design approach. The required high reliability and lack of prototypical testing have resulted in the development of high-fidelity Multiphysics simulation methods in which coupling between fluid flow, heat transfer, and structural mechanics is essential. Additionally, prediction of failure modes cannot traditionally be made at the macroscopic level since sub-microscopic defects can emerge suddenly in localized structural zones. This realization has propelled the interest in the development of Multiscale methods of analysis once the Multiphysics design is optimized. Thus, Multiphysics is a design tool, while Multiscale is a failure assessment tool. We present here recent progress on the implementation of a tightly-coupled Multiphysics-Multiscale procedure for the specific purpose of designing high heat-flux components in severe environments. The focus of the presentation will be on a new variational method for embedding smaller length scale Representative Volume Elements (RVEs) into increasingly larger domains, where the mismatch in displacements and tractions is minimized at the interfaces. At the larger length scale, an elastic solution is first developed to identify critical zones in which continuum elasto-plasticity is required. Another RVE of a continuum elasto-plastic model is embedded, and the variational principle is used to guarantee a smooth translon across the interface region, since the constitutive equations are not the same. Further embedding of smaller RVEs will be shown, where we used a dislocation-based crystal plasticity model to resolve plastic deformation and its dependence on microstructural details. Finally, discrete dislocation dynamics is used to determine rates of dislocation generation and reactions in the crystal plasticity model.

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