VIRTUAL SIMULATION AND DESIGN OF BARRIER COATINGS FOR CERAMIC COMPOSITES

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The development of environmental barrier coating systems for ceramic composites has two central challenges: (i) the selection of materials and layer architectures that are resistant to cracking, volatilization, and chemical attack, and (ii) the identification of active failure mechanisms and their dependency on the system's intrinsic properties. This talk will describe two modeling frameworks that are tailored to these two objectives.

In the first framework, an automated approach for analyzing delamination and mud-cracking in complex multilayers enables developers to consider a broad range of materials and architectures and in turn rapidly identify promising material systems. The opportunities created by this framework will be demonstrated by illustrating the likely failure modes of environmental barrier coatings comprising multiple layers of rare earth silicates on silicon carbide substrates. These map illustrate combinations of material properties (e.g. coating thickness and thermal expansion coefficients) that avoid penetrating mud cracks and delamination cracks. Maps will also be presented that quantify the likelihood of crack kinking, i.e. the transition of a penetrating crack to a delamination crack that leads to coating failure.

In the second framework, distributed cohesive zone models are used to develop a virtual testing framework: the framework is capable of predicting a broad range of cracking modes without a priori assumptions regarding the failure mode and without phenomenological criteria for the evolution of damage. In this framework, cracks emerge from defects in the structure according to classical brittle fracture theory. The simulation framework exploits highly parallel computing approaches that enable simulations covering a broad range of parameter space; this enables the construction of "durability regime maps", which indicate likely failure mechanisms as a function of material properties. This framework has been used to identify whether or not interface cracks will travel along an interface or kink into the coating (leading to spallation), as a function of interface toughness, film toughness, mixed mode loading, and interface waviness. The results shed new light on the physics of crack kinking, which plays a fundamental role in coating durability. Further, the results provide insights regarding the role of interface waviness between coatings and substrates, such as would occur with a coated woven textile composite.