COMPUTATIONAL TOOL TO ACCELERATE CMAS-RESISTANT TBC DESIGN FOR AERO-TURBINE APPLICATIONS

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Key Words: CMAS, TBC design, CALPHAD, thermodynamics, ICME

Infiltration of molten Calcium-Magnesium Alumino-Silicate (CMAS) deposits is a primary cause of failure of thermal barrier coatings (TBCs) on aero-turbine engine blades. Cooling of infiltrated CMAS deposits leads to densification and subsequent cracking and delamination driven by internal strain energy due to the thermal mismatch between the solidified CMAS melt and the porous columnar TBC architecture. Infiltration kinetics, and thus onset of mechanical failure, are strongly affected by the thermodynamic properties of the CMAS melt (viscosity, melting point, etc.) and the crystalline reaction products formed due to the interaction between the CMAS melt and TBC material, which can block the channels in the TBC structure and inhibit further melt infiltration. Additional complexity is added due to the wide range of CMAS deposit compositions found in nature, which can lead to vastly disparate melt behavior and CMAS-TBC reactivity dependent on both deposit and coating composition.

A robust model to predict TBC failure and enable the design of novel CMAS-resistant TBC materials therefore relies on the ability to model CMAS melt properties and the reactivity between melt and coating. A computational design tool is currently under development to enable Integrated Computational Materials Engineering (ICME)-informed modeling of CMAS-TBC interaction and coating performance. This computational tool leverages Calculation of PHase Diagram (CALPHAD)-based thermodynamic databases which include the components of CMAS-Fe deposits as well as RE zirconate (RE=Y,Gd) TBC materials. A tool framework compatible with the Thermo-Calc software will allow for wide availability of the design tool across academic and industrial R&D communities. The tool enables TBC design by streamlining thermodynamic calculations related to CMAS melt properties and CMAS/TBC reactivity, feeding results into property and performance models. A CMAS selection module contains a compiled list of CMAS compositions while also allowing for user-defined compositions, allowing for quick assessment of CMAS melt properties across relevant deposit compositions and ranges. Efficient comparison of CMAS/TBC interactions can be performed across a large number of pre-defined or user-defined CMAS chemistries. CMAS reactivity may also be assessed across a range of RE/Zr ratios as well as compared between various RE systems. Examples of tool functionalities and relevant thermodynamic calculations will be presented. Future work includes integration with thermomechanical and kinetic infiltration models to predict TBC performance.