OXIDATION OF HIGH-ENTROPY ULTRA-HIGH TEMPERATURE CERAMICS

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High entropy borides and carbides are a relatively new class of UHTCs. Computational and experimental investigations were utilized to understand oxidation of constituents within equimolar, five-component solutions MX, where M consisted of (Hf,Zr,Ti,Ta,Nb) and X was C or B₂. Thermodynamic calculations conducted using FactSage software and databases predicted oxidation products of the constituent borides and carbides wherein Group IV (Hf,Zr,Ti) oxides dominated the oxide scale, resulting in a Group V (Ta,Nb) enriched substrate. These predictions were verified at the substrate-oxide interface for material exposures conducted at temperatures of 1500°C-1800°C in 0.1 to 1% O₂ balance argon, as shown in the figure below. The surface oxides, however, consisted of an assemblage of all the oxides resulting in the formation of nonprotective low melting eutectics. Additional experiments conducted with (Hf,Zr,Ti,W,Mo) (Group IV + VI) carbides demonstrated that the formation of less thermodynamically stable and gaseous oxides WO₃ and MO₃ did not result in eutectic melts and slower material consumption rates were observed.



Cross-section SEM/EDS of (HfZrTiTaNb) B_2 oxidized at 1700 °C in 1%O₂/argon for 5 min. Region shown is 3 mm below the oxide/gas surface. Note the preferential oxidation of Hf and Zr leaving Ta and Nb in the boride. Ti is partially oxidized.