THEORETICAL PREDICTION ON ROOM AND HIGH TEMPERATURE MECHANICAL AND THERMAL PROPERTIES OF THE MATRIX AND INTERPHASE MATERIALS FOR FUTURE UHTC_F/UHTC COMPOSITES

Yanchun Zhou, Science and Technology on Advanced Functional Composite Laboratory, Aerospace Research Institute of Materials & Processing Technology, China yczhou@imr.ac.cn

Huimin Xiang, Science and Technology on Advanced Functional Composite Laboratory, Aerospace Research Institute of Materials & Processing Technology, China

Fu-zhi Dai, Science and Technology on Advanced Functional Composite Laboratory, Aerospace Research Institute of Materials & Processing Technology, China

Key Words: Ultrahigh-temperature ceramics; Composites; Interphases; DFT calculations; Thermal and mechanical properties.

Ultrahigh-temperature ceramics (UHTCs) are materials of choice for future hypersonic vehicles as nose tip and sharp leading edges, as well as hot structure components for scramjet engines. However, the brittleness and poor thermal shock resistance are prevailing problems that have blocked the real applications of the current UHTCs. To overcome the brittleness and poor thermal shock resistance, ultrahigh-temperature ceramic fiber reinforced ultrahigh-temperature ceramic matrix (UHTC_f/UHTC) composites must be developed. The advantages of future UHTC/UHTC composites include excellent defect tolerance, high fracture toughness, low density, excellent thermal shock resistance, and high thermal conductivity. Recently, high ceramic yield liquid UHTC precursors and UHTC fibers have been developed, which enable the design and fabrication of UHTC_f/UHTC composites utilizing a combined process of CVI and PIP. As for other CMCs, in designing future UHTC_f/UHTC composites, fiber-matrix interphase is apt to play a determining role to ensure load transfer, fiber pull-out, and toughening. However, the interphase materials for future UHTCt/UHTC composites are not available yet. In this talk, the room and high temperature mechanical and thermal properties of TMB₂ (TM=transition metals) investigated by a combination of first principle and phonon dispersion calculations will be presented first. Then the criteria and methods for searching for the promising interphase materials of UHTC_f/UHTC composites including "soft" transition metal borides and borocarbides will be presented. Finally, the chemical bonding nature that underpins the properties of these materials will be discussed. Methods to strengthen the grain boundary of UHTC_f will be proposed. And the effect of weak t bond formed by the overlapping of perpendicular p orbitals on the mechanical properties is emphasized.