

**PhD Comprehensive Exam Announcement**  
**Mechanical and Aerospace Engineering Department**  
**University of Texas at Arlington**

**MOLECULAR LEVEL MECHANICAL PROPERTIES OF ULTRA HIGH  
TEMPERATURE CERAMICS AND THEIR NANOCOMPOSITES**

**By**

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**Abstract**

In this study, we propose that selective nanoparticle reinforcement may assist in achieving tailored mechanical properties of ultra-high temperature ceramics. To support our hypotheses, we performed preliminary studies to evaluate the mechanical behavior of ultra-high temperature ceramics and their nanocomposites. Two different material systems have been studied, namely the  $ZrB_2$ -based and the  $HfO_2$ -based nanocomposites. First, the atomistic models of the polycrystalline  $ZrB_2$  and  $ZrC-ZrB_2$  nanocomposites were subjected to tensile loading to determine their elastic constants and tensile strengths. It was found that the presence of nanoparticles imparts an insignificant effect on the mechanical properties of  $ZrB_2$ . It has also been observed that the failure mechanisms of both the  $ZrB_2$  and  $ZrC-ZrB_2$  nanocomposite are driven by grain boundary deformation. For the  $HfO_2$  based system, the material's tensile properties are evaluated at different temperatures and different electric field conditions. The study shows that the residual stress developed due to the electric field could be a factor in degrading diffusion property of  $HfO_2$ . Through these preliminary studies, the key parameters contributing to the mechanical properties of the UHTCS are identified. Future studies will include the effect of these parameters on the overall mechanical properties of UHTCS.