Multiscale computer simulation dynamic fracture of ultrahigh temperature ceramics at room and elevated temperatures

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Abstract

Multiscale computer simulation approach has been applied to research mechanisms of failure in ultra-high temperature ceramics under dynamic loading at room and temperatures below 1500 K.
The ultra-high temperature ceramics (UHTC) based on zirconium diboride, titanium diboride, hafnium diboride, zirconium carbide, hafnium carbide, tantalum carbide constitute a class of promising materials for high temperature applications in the aerospace industry for hypersonic re-entry vehicles, rocket nozzle inserts, and cutting tools, wear resistant parts etc. The goal of this work is study the dynamic strength and dynamic toughness of several types UHTC, as well as the study of physical mechanisms of quasi-brittle fracture by the method of multilevel computer simulation. The complexity of prediction of mechanical properties of massive UHTC constructive elements caused with influence of residual stress, residual porosity and grain size distribution in ceramics on damage nucleation and growth. A presence of pores in ceramics leads to the reduction of fracture toughness, modulus of elasticity and strength. The computational models of a structured representative volume (RVE) of UHTC were developed using the data of structure researches of specimens manufactured by a hot pressed and a selective laser sintering. Distribution of residual thermal stress after manufacturing were estimated in assumption that temperature drop can varied within the range of 1100 K to 1600 K. Critical fracture stress under compression of mesoscale level depends not only on relative volumes of voids and inclusions, but also on its size distribution. Damage of UHTC nanocomposites can be originated under stress pulse amplitude less than the Hugoniot elastic limit of matrix. The dynamic strength under tension (the spall strength) of UHTC nanocomposites depends on relative volumes and sizes of voids and inclusions. The decreasing of the shear strength can be caused by local stresses due to a several factors such as residual thermal stresses, nano-voids near triple junctions of ceramics matrix grains, penny-shaped cracks. Results of computer simulation indicate quasi-brittle fracture of UHTC ceramics under dynamic compression and tension. The process of quasi-brittle fracture in UHTC composites is probabilistic in nature. Damage nucleation and accumulation in quasi brittle nanostructured UHTC takes place under shock compression. Fracture of nanostructured UHTC under pulse and shock-wave loadings is provided by fast processes of intercrystalline brittle fracture and relatively slow processes of quasi-brittle failure via growth and coalescence of opened microcracks. The influence of residual stresses on the growth of micro and microcracks under dynamic loading of UHTC ceramics decreases at temperatures from 800 to 1500 K. Results of simulations showed that the Hugoniot elastic limit of ZrB_2-15 vol. % B_4C at 1200 K is higher on 10 % in comparison with the value at room temperature.

Keywords: Multiscale simulation, dynamic fracture, UHTC, high temperatures