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Thermal Stress in a Zero Thermal Expansion Composite

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Abstract

Introduction:
Zirconium tungstate, ZrW2O8, is a material which possesses a negative coefficient of thermal expansion over a wide temperature range (0.5 to 1050 K) [1]. There is interest in using ZrW2O8 in composites to create an effective zero thermal expansion material. The ZrO2-ZrW2O8 composite system has been studied, and several composites with varying microstructures and pore fractions have been reported in the literature [2]. Thermal stress upon cooling could cause material failure and a pressure-induced first-order phase transition in ZrW2O8 which could both increase the overall coefficient of thermal expansion and reduce the sample integrity. Our earlier finite element analysis of the composite without pores predicted high thermal stresses upon cooling [3], and the present analysis aims to extend that study to porous materials, to investigate ways to manage thermal stress by changing the microstructure.
Use of COMSOL Multiphysics:
A series of 2-D finite element models of a ZrO2-ZrW2O8 composite system were created in COMSOL Multiphysics to study the effect of pores between the matrix (ZrO2) and filler (ZrW2O8) materials (Figure 1). Pores were modeled as ellipses concentric with the filler particles. Seventeen model geometries of varying microstructure were studied in order to determine correlations between microstructural factors and thermal stress. A contact model of closing pores was included. A hyperelastic material model was created to determine the effects of the pressure-induced phase transition.
Results:
Increased porosity was found to correlate with decreased compressive stress in the filler particles and decreased progress of the pressure-induced phase transition. Very high compressive and tensile thermal stresses were predicted by the model, especially near thin crack-like areas of the pores (Figure 2). The closure of pores significantly changed the stress distribution, as local stress maxima became local stress minima. The hyperelastic model predicted a change of the stress in the filler particle from compressive to tensile as the pressure-induced phase transition proceeds.
Conclusions:
To protect sensitive filler particles from thermal stress while maintaining the overall strength of the composite, it might be desirable to create materials with small pore volumes and small matrix-filler interfaces. The pressure-induced phase transition of ZrW2O8 is in some ways beneficial as it acts as a strain energy sink and counteracts tensile stress in the matrix, but it could lead to substantial other changes.

Reference

1. T.A. Mary et al, Negative Thermal Expansion from 0.3 to 1050 Kelvin in ZrW208, Science, 272, 90-2 (1996)
2. Li Sun et al, ZrW2O8-containing composites with near-zero coefficient of thermal expansion fabricated by various methods: Comparison and optimization, Composites Science and Technology, 68, 3425–30 (2008)
3. Michael Jakubinek et al, Negative thermal expansion materials, Journal of Thermal Analysis and Calorimetry, 99, 165-72 (2010)

Figures used in the abstract

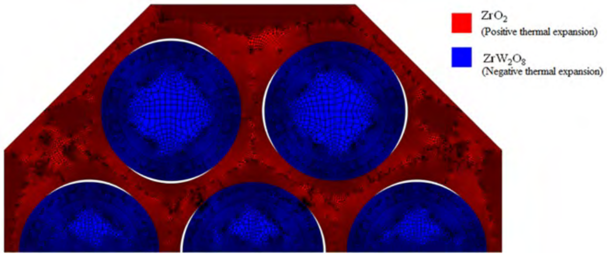

Figure 1: A meshed model geometry. Mismatch between the coefficients of thermal expansion of the matrix (ZrO2) and filler (ZrW2O8) materials creates thermal stress.

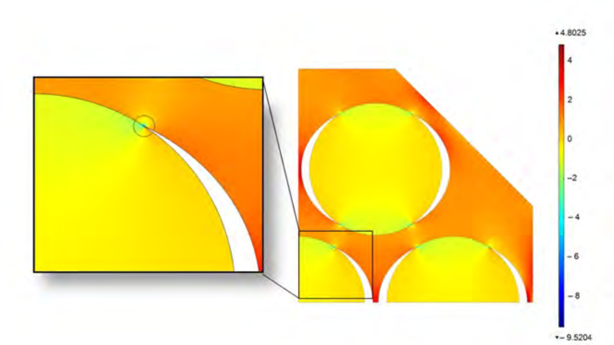

Figure 2: The distribution of the first principal invariant of stress in GPa in a representative model. Anisotropy in the stress distribution in the filler particles is caused by the pores.