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CHARACTERIZATION OF RESIDUAL STRESSES IN GRADED CERAMIC-METAL STRUCTURES: A COMPARISON OF DIFFRACTION EXPERIMENTS AND FEM CALCULATIONS

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1. INTRODUCTION

Numerical models have been extensively developed for predicting the thermomechanical behavior of ceramic-metal joints containing graded interlayers. The goal of such modeling is to be able to design optimum interlayer microstructural characteristics required to meet the needs of specific application conditions, and to use this design information to guide component fabrication. In order to have confidence in the outcome of these modeling efforts, it is critical that the models be validated by comparison with experimental results, at least for some model systems and simple specimen geometries. In this study, residual strain and stress distributions are being studied using a combination of FEM calculations and diffraction techniques.

The graded specimen examined in this research was fabricated by powder processing methods. Al_2O_3 -Ni was selected as a model system. The residual stresses expected in the specimen were predicted by FEM calculations using an elastic-plastic model. Strain and stress distributions in the specimen were characterized experimentally using x-ray and neutron diffraction techniques. In this paper, preliminary experimental results are presented and compared with model predictions.

2. EXPERIMENTAL

2.1 Specimen Fabrication

The steps involved in the production of the graded Ni- Al_2O_3 specimen included powder selection, incorporation of sintering aids and binders, mixing desired powder compositions, layering powders in a die, compaction, debinding and sintering, and final consolidation by hot isostatic pressing (HIP). Details of the specimen preparation have been presented previously [1,2].

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Figure 1 shows the cylindrical Ni-Al₂O₃ specimen examined in these experiments, along with the microstructures within the graded interlayer. The joined specimen was approximately 40 mm in length and 9 mm in diameter. Intermediate stepwise compositions of 20, 40, 60 and 80 vol.% Ni were used, and the joint was linearly graded over a thickness of approximately 12 mm. Note the distinct transition in microstructure that has been achieved in the composite interlayers by controlling the starting Al₂O₃ and Ni particle sizes during fabrication. Specifically, the 20 and 40 vol.% Ni layers (fabricated using 0.5 μ m Al₂O₃ and 18 μ m Ni) exhibit a continuous ceramic matrix with dispersed metal particles, whereas the 60 and 80 vol.% layers (fabricated using 22 μ m Al₂O₃ and 5 μ m Ni) exhibit a continuous metallic matrix with dispersed ceramic particles. The use of a submicron ceramic particle size in the ceramic-rich layers is necessary to achieve adequate densification of these composites, and the change to a large ceramic:metal particle size ratio in the metal-rich layers allows a continuous metal matrix to be obtained in these composite microstructures.

2.2 FEM Modeling

Continuum models were used to compute residual stresses and strains developed in the joined Al₂O₃-Ni specimen during simulated cooling from 1100 K to room temperature. Figure 2 shows the specimen geometry and mesh used in the analysis. Because both the specimen and its loading (thermal) are axisymmetric, it is possible to restrict models to two dimensions. Spatially uniform cooling was assumed, thus only the equations of stress equilibrium need to be solved. The graded region was treated as a series of four perfectly bonded composite interlayers, each layer being assigned different material properties. Material behavior was assumed to be independent of time (no creep). The Al₂O₃ was assumed to remain elastic, with plasticity permitted within the Ni and any interlayer materials; a von Mises yield condition and isotropic hardening were utilized.

Figure 1. Photograph showing the graded Al₂O₃-Ni specimen examined in this study along with the microstructures observed within the graded interlayer.

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Stress-strain constitutive parameters for composite interlayers were computed using a modified rule-of-mixtures approach using temperature dependent mechanical property and thermal expansion values. Details of the FEM model, including assumptions regarding constitutive behavior, have been presented previously [2-4]. Numerical solutions were obtained using the ABAQUS finite element computer program [5].

2.3 Diffraction Measurements

Elastic strains were measured along the surface and within the interior of the specimen using x-ray and neutron diffraction techniques, respectively. The x-ray measurements were based on the well known "sin²ψ method" [6]. Figure 3 shows the coordinate system used. Referring to this figure, the general equation for strain measurement can be expressed as

$$(\epsilon_{33})_{\phi,\psi} = \frac{d_{\phi,\psi} - d_0}{d_0} = \epsilon_{11} \cos^2 \phi \sin^2 \psi + \epsilon_{12} \sin 2\phi \sin^2 \psi + \epsilon_{22} \sin^2 \phi \sin^2 \psi + \epsilon_{33} \cos^2 \psi + \epsilon_{13} \cos \phi \sin 2\psi + \epsilon_{23} \sin \phi \sin 2\psi \quad (1)$$

which for an isotropic material allows stresses to be calculated according to

$$(\epsilon_{33})_{\phi,\psi} = \frac{d_{\phi,\psi} - d_0}{d_0} = \frac{1+\nu}{E} (\sigma_{11} \cos^2 \phi + \sigma_{12} \sin 2\phi + \sigma_{22} \sin^2 \phi - \sigma_{33}) \sin^2 \psi + \frac{1+\nu}{E} \sigma_{33} - \frac{\nu}{E} (\sigma_{11} + \sigma_{22} + \sigma_{33}) + \frac{1+\nu}{E} (\sigma_{13} \cos \phi + \sigma_{23} \sin \phi) \sin 2\psi \quad (2)$$

Residual strains within the pure Al₂O₃ result from the thermal expansion mismatch between the Al₂O₃ and the remainder of the structure to which it is joined. Within the composite interlayers, however, both macro- (between layers) and microstrains (between phases) exist. According to Noyan and Cohen [6], the total strain measured within each phase of the composite is the sum of the macro- and micro- components, such that, in the case of Ni for example

$$\sigma_{ij}^T(\text{Ni}) = \sigma_{ij}^m + \sigma_{ij}^\mu(\text{Ni})$$

Macro stresses are the same for both phases in the composite, however, micro stresses must be balanced according to

$$(1-f)\sigma_{ij}^\mu(\text{Al}_2\text{O}_3) + f\sigma_{ij}^\mu(\text{Ni}) = 0$$

Figure 2. Specimen geometry and mesh used in the FEM calculations.

Since the FEM model we have adopted predicts only macro stresses, experimental data taken from composite layers must be separated into macro- and micro- components using

Figure 3. Coordinate system used for diffraction experiments.

the above equations. In the neutron diffraction experiments, a sampling volume of 1 mm x 1 mm x 1 mm was used. Since only the Al_2O_3 was examined, it was not possible at this time to separate the macro- and micro- components from the neutron data.

3. RESULTS AND DISCUSSION

Since failure in ceramic-metal joints of this geometry typically results from crack propagation within the ceramic adjacent to the bonded interface, attention was focused on this region of the specimen. Data was collected from within the pure Al_2O_3 and only the first few composite interlayers. Results are reported in terms of specific strain or stress components for the interior of the specimen (neutron measurements) or along the surface of the cylindrical specimen (x-ray measurements).

The most critical stress responsible for causing fracture is the axial tensile stress within the Al_2O_3 along the surface of the specimen. Figure 4 shows this stress component as measured by x-ray diffraction and as predicted by FEM modeling. For both the modeling and experimental results the peak tensile stress exists within the Al_2O_3 close to the interface between the Al_2O_3 and the 20% Ni composite layer. Note that the magnitude of the peak stress measured experimentally is significantly lower than that predicted by the model. The peak value predicted by the model can be made to agree more closely with the experimental value by taking into account porosity effects on Al_2O_3 properties and creep effects within the Ni [7]. Within the composite interlayers the macrostress measured experimentally shows cyclic variations similar to those predicted by the model, however, close agreement between the measured and predicted values

Figure 4. X-ray diffraction results measured along the specimen surface showing the axial stress as a function of position. The FEM prediction is shown for comparison.

Figure 5. Neutron diffraction results showing the radial strain measured along the axis of symmetry as a function of position. The rms microstrain calculated from peak broadening is also shown.

was not obtained.

Figure 5 shows the radial strains measured by neutron diffraction along the centerline of the specimen, as well as the rms microstrain determined from a simple line broadening analysis. The following observations can be made regarding this data. First, the magnitudes of the strains are quite small, in all cases less than 5×10^{-4} . Secondly, and perhaps most importantly, tensile radial strains were experimentally observed within the Al_2O_3 , whereas, since the ceramic has a lower coefficient of thermal expansion than the metal, these strains are expected to be compressive. The rms microstrain is very low in the pure Al_2O_3 and increases within the 20% and 40% Ni composite interlayers.

Finally, Figure 6 shows the axial strain within the Al_2O_3 as a function of radial position measured at a location 0.7 mm from the interface between the pure Al_2O_3 and the 20% Ni composite layer. Starting from the axis of symmetry and moving outward toward the radial free edge the axial strain was observed to be quite low, as predicted by the FEM model. However, very close to the radial free surface the model predicts a rapid increase in tensile strain which could not be observed experimentally due to the limited practical spatial resolution of the neutron diffraction sampled volume.

Figure 6. Neutron diffraction results showing the axial strain as a function of radial position within the pure Al_2O_3 at a location 0.7 mm from the Al_2O_3 /FGM interface.

The reasons for the apparent disagreement between the experimental results and the FEM predictions are not clear at this time. In the case of the lower axial stress within the Al_2O_3 measured by x-ray diffraction on the specimen surface (Figure 4), there are always questions regarding the validity of the constitutive assumptions used in the FEM model that could account for this discrepancy. Other potential explanations include possible microcracking stress relief within the ceramic, or the influence of surface preparation. Regarding the radial strain along the axis of symmetry (Figure 5), however, the apparent existence of tensile strains within the Al_2O_3 is more puzzling. It would seem that this result would only be possible if the thermal expansion coefficients did not vary with volume fraction in a monotonic fashion, as would be expected from the rule-of-mixtures. Detailed characterization of the expansion coefficient and mechanical properties (elastic modulus and yield strength) of the individual composite materials used as interlayers is now being performed in an effort to address these questions. In addition, neutron and x-ray diffraction experiments will be carried out in the future on a single composite interlayer joint (e.g. 60% Ni) in which the stress and strain distributions are expected to be less complicated.

4. CONCLUSIONS

The residual strains and stresses in a powder processed axisymmetric Al_2O_3 -Ni graded specimen have been characterized by a combination of numerical and experimental techniques. Preliminary neutron and x-ray diffraction measurements were not in very good agreement with FEM model predictions, particularly regarding the in-plane stresses along the axis of symmetry. These results suggest additional diffraction measurements on graded specimens having fewer interlayers should be carried out, and experimental verification of the constitutive assumptions used in the FEM model is needed.

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