PREDICTION OF CARBON-CARBON COMPOSITE THERMOELASTIC PROPERTIES USING X-RAY DIFFRACTION DATA

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Introduction

The thermoelastic moduli of most composites can be computed using classical micromechanical models, provided the moduli and coefficients of thermal expansion (CTE) of the constituents, details of the fiber architecture and fiber volume fraction, etc. are known. Frequently with carbon-carbon (C-C) composites, due to the high heat treatment temperatures used in the fabrication process and the fact that constituents' properties change with heat treatment, the individual constituents' thermoelastic properties are not known. In an attempt to estimate the in-situ properties of C-C constituents following fabrication, X-ray diffraction (XRD) data of several different carbon-carbon (C-C) composites and on reinforcement subjected to the same graphitization temperatures was measured by the Aerospace Corporation and used by the author within submicromechanical mathematical models to predict the thermoelastic moduli of the C-C constituents. Composite characterization data, e.g. density, fiber architecture, fiber volume fraction, etc. measured by the Aerospace Corporation, Southern Research Institute (SRI), and the C-C fabricator, were used in micromechanical and multidirectional composite models to predict the C-C composite properties. Moduli and CTEs of the composites, measured by SRI, enabled a correlation between predicted and measured moduli to be performed.

Characterization Data

Two different types of C-C composites were examined in this study. The first type was fabric reinforced in which non-thermally stable fibers (Amoco's P-30X and Mitsubishi Kasei's K321) provided reinforcement for a pitch matrix composite. The second type consists of Amoco's Self Reinforced Graphite (SRG) in a quasi-unidirectional orientation also densified with pitch-based matrix material. For both types of composites, graphitization temperatures well in excess of 2000°C were used. For the fabric reinforced composites, during the graphitization step witness fabric was placed in the furnace with the composites to insure that it experienced the same temperatures for the same duration as the composites themselves. In this way, XRD data measured on the fabric alone is as representative of the structural characteristics of the fiber in the composites as is possible. Since the SRG experiences temperatures during its fabrication which are as high as that experienced by the SRG/carbon composites, the placement of witness SRG within the graph furnace was deemed unnecessary.

For the fabric reinforced composites, the Aerospace Corporation measured average crystallite domain lengths (L_a, L_c), and interlayer spacing (d_{002}) on both the composites and on the witness fabric. For the SRG/carbon composites, the average domain lengths and interlayer spacing were measured on the composites. Earlier measurements on undensified SRG by the Aerospace Corporation [1] were used to obtain structural characteristic of the SRG representative of that in the SRG/carbon composites. Table 1 provides a summary of the composite and reinforcement XRD data.

Table 1. Summary of Aerospace Corporation XRD data.

Compos	Composite XRD			Fiber XRD		
	L_a nm	L_c nm	d_{002} nm	L_a nm	L_c nm	d_{002} nm
K321/C	58.5	38.0	.3372	50.5	32.5	.3376
P30X/C	52.0	38.0	.3372	48.6	32.5	.3375
SRG/C	90.5	61.8	.3366	78.5	58.5	.3366

This XRD data indicates that the K321 fibers and composites have longer crystallite domain lengths in the fiber axis direction (L_a), indicating that the K321 fibers very likely have a higher axial Young's modulus than the P-30X fibers for the same graphitization conditions. It is also apparent from Table 1 that the SRG reinforcement and its composites are extremely stiff materials. One other important item from Table 1 is that composite graphitization is shown to be more extensive than that of the fiber alone. This indicates that the matrix will be highly graphitized and therefore contribute substantially to the composite stiffness.

Standard characterization data for these composites, as measured by the fabricator and SRI, includes fiber volume fraction from areal weights, densities, and checks on fiber orientation. The summary of composite characterization data is provided in Table 2.

Table 2. Summary of composite characterization data.

Composite	Architecture	Fiber Volume Fraction	Density (g/cc)
K321/C	0/90 1:1 0/90 4:1	.52 .49	1.84 1.79
P30X/C	0/90 1:1 0/90 4:1	.49 .48	1.78 1.76
SRG/C	±2.5°	.78	1.85

Results and Discussion

The measured fiber L_a values were first used to compute the thermoelastic moduli of each of the three fibers. This was accomplished by means of submicromechanical models [2] starting at the graphite crystal level and building to a model of the fiber itself, based on crystallite orientation distributions and expected crystallite textures within the fiber cross-section. Next, by means of a rule of mixtures approach, the composite L_a values were used to back calculate matrix L_a values using the measured fiber L_a, obtained directly from the witness reinforcement. Matrix moduli calculated in that fashion proved to be much too high relative to measured composite properties. Micromechanical models [3] and experience with these composites have shown substantial degradation in effective thermoelastic moduli in anisotropic phases with the extent and orientation of cracking typical of that occurring in 2-D C-C. No crack mapping was performed or recommended in this study. It was decided that the back calculation of the matrix moduli would be performed instead. However, due to the large matrix L_a, a high matrix modulus is still anticipated despite the cracking and porosity. The effective matrix moduli of the cracked and porous P-30X 1:1 C-C was calculated from the measured data. In all subsequent C-C composite property calculations, matrix moduli were adjusted for different levels of porosity, treating pores as cylindrical voids. Thus the process for all composites after the P-30X C-C was to calculate the fiber moduli using the fiber L_a and determine matrix moduli by modifying the baseline (P-30X C-C) matrix for the appropriate void volume.

The degree of correlation between the measured and calculated P-30X composite properties is, by definition, essentially exact. The level of correspondence obtained for the K321 C-C, using the approach outline above, is indicated in Figure 1. The relative agreement between measured and calculated CTEs is shown in Figure 2. Excellent agreement has been obtained.

Compressive stress-strain curves for the SRG/carbon composites show a very highly nonlinear nature, which is believed to be evidence of a scissoring effect within the SRG tows. After accounting for this, the models were successfully used to calculate the CTE's and other (e.g. shear) moduli.

Conclusions

Measured XRD data on C-C composites and on witness reinforcement has provided valuable data for determining the relative participation of the C-C constituents in the composite properties. The matrix values were found to be substantially affected by cracking and porosity but nevertheless very significant, substantially higher than those of an ATJ-like isotropic matrix. The XRD data has proven to be indispensable in the calculation of the C-C constituent properties. The validity of the models has been demonstrated by the correlation of calculated and measured conductivities.

References

1. P. Adams, Aerospace Rpt.# ATR-96(1970)-1, 1/96.
2. B.W. Rosen and B.J. Sullivan, Extended Abstracts, 19th Biennial Conf. Carbon, 1989, pp. 300-301.
3. B.J. Sullivan, 14th Conference on Metal Matrix, Carbon, and Ceramic Matrix Composites, Cocoa Beach, FL, 1990, pp.327-343.

Figure 1.

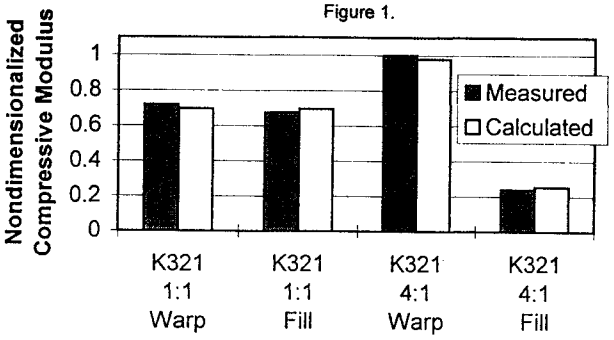

Figure 2.