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QUANTIFYING UNCERTAINTIES IN THE THERMO-MECHANICAL PROPERTIES OF PARTICULATE REINFORCED COMPOSITES

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ABSTRACT

The present paper reports results from a computational simulation of probabilistic particulate reinforced composite behavior. The approach consists of simplified micromechanics of particulate reinforced composites together with a fast probability integration (FPI) technique. Sample results are presented for a Al/SiC_p (silicon carbide particles in aluminum matrix) composite. The probability density functions for composite moduli, thermal expansion coefficient and thermal conductivities along with their sensitivity factors are computed. The effect of different assumed distributions and the effect of reducing scatter in constituent properties on the thermal expansion coefficient are also evaluated. The variations in the constituent properties that directly effect these composite properties are accounted for by assumed probabilistic distributions. The results show that the present technique provides valuable information about the scatter in composite properties and sensitivity factors, which are useful to test or design engineers.

1. INTRODUCTION

Particle reinforced composites are being used in a wide variety of aerospace and non-aerospace applications. The high costs and technical difficulties involved with the fabrication of fiber-reinforced composites often limit their use in many applications. Consequently, particulate reinforced composites have emerged as viable alternatives to conventional fiber reinforced composites. These composites can be processed to near net-shape and have improved stiffness, strength and fracture-toughness characteristics. Particle reinforced composites can also be used as matrix materials in continuous fiber reinforced composite materials. They are potential candidate materials where shock or impact properties are important. Particle reinforced metal matrix composites have shown great potential in a variety of automotive applications. Typically, these materials are aluminum matrix reinforced with SiC or TiC particles. The resulting material has high specific modulus and strength which makes it suitable for disk brake rotors, connecting rods, cylinder liners and other high temperature applications.

The characterization of these materials is fundamental to their reliable use. A set of micromechanics equations has been developed for prediction of thermal and mechanical properties of particulate reinforced composites [1]. These simplified equations are based on mechanics of materials approach and can easily account for environmental effects such as moisture or temperature. However, the overall composite properties exhibit scatter due to the uncertainties in constituent material properties, constituent volume fractions and fabrication-related parameters. Consequently, there is a need for analytical tools that formally account for these uncertainties and quantify the overall composite behavior.

The observed scatter in the global composite behavior or "response", is usually due to the existence of uncertainties in the basic or "primitive" variables. Primitive variables are properties/parameters that participate at the lowest level (e.g. at the micromechanics level) in defining a global property. The fiber volume fraction, individual constituent properties such as moduli, thermal expansion coefficients, heat conductivities, and strengths are examples of primitive variables. These are assumed to be independent and have their own statistical distributions. Response variables are those that characterize the composite behavior, such as the composite moduli, thermal conductivities, and thermal expansions coefficients.

The approach to quantify probabilistic composite behavior combines the micromechanics of particulate reinforced composites with a fast probability integration (FPI) technique [2]. The role of micromechanics equations was to provide functional relationships (micromechanics and macromechanics) that tie the constituent properties to the equivalent composite behavior. The role of FPI was to perform probabilistic analyses by utilizing the properties generated by the micromechanics equations. The combined procedure yields probabilistic distribution, and density functions of the global composite properties. Furthermore, the procedure also identifies and ranks the sensitivities of the various primitive variables on the global composite property and its scatter.

The objectives of the present work are to develop a computational technique to quantify the scatter in particulate reinforced composite properties via formal probabilistic analyses and illustrate the methodology with typical results for a specific particle reinforced metal matrix composite. The results are presented in the form of probability density functions (PDF) for the composite normal and shear modulus, thermal expansion coefficient and thermal conductivity. . A PDF is the relationship defined by the value of a property to its probability of occurrence. Also presented are the corresponding sensitivity factors, which are obtained as by products of FPI technique. In addition, a separate study is conducted whereby the effect of different assumed distributions of constituent properties as well as the reduction of scatter in those input variables on composite thermal expansion coefficient are also shown.

2. PARTICULATE COMPOSITE MICRO-MECHANICS

A set of micromechanics equations was developed for particulate reinforced composites along the same lines as those for continuous fiber reinforced composites. A brief summary of these equations will be provided here. Detailed description is provided elsewhere [1]. The particulate matrix material is assumed to be uniformly dispersed with spherical particles. This is analogous to the assumption of regular "array pattern" for fiber reinforced composites. The diameter of the particles is assumed to be the average value of the range of diameters in a cubic lattice. The distance between the particles is computed from the overall particle volume fraction. Hence, one can think of a representative volume element (RVE) or a "unit cell" as shown in Fig. 1(a). In order to facilitate the definition of certain micro-regions and to compute microstresses, the spherical particle has been replaced by a cubic particle of the same volume as shown in Fig. 1(b). The RVE now becomes a three-dimensional entity. A list of assumptions implicit in the micromechanics of particulate composites are given below:

1. The composite is composed of two-phases - particles and binder (matrix).
2. Each phase of the composite can be described by the continuum mechanics. Hence, the input parameters are moduli, Poisson's ratios, thermal expansion coefficients, thermal conductivities etc. of each individual phase.
3. The interface between the particle and the binder has been assumed to be a perfect bond.
4. The micromechanics is characterized by average values of composite properties and average constituent stresses over a certain region.
5. The properties of individual phases are assumed to be isotropic.

As mentioned before, only select equations will be shown here without any derivation of those equations. The following is a brief list of various equations:

The mass density of the particulate composite is given by

$$\rho_{pc} = V_f \cdot \rho_p + (1 - V_f) \cdot \rho_b \tag{1}$$

where V_f is the volume fraction of the particles, subscripts pc, p and b stand for particulate composite, particle and the binder, respectively.
The normal modulus is given by -

$$E_{pc} = \frac{V_f^{0.67} E_b}{1 - V_f^{0.33}\left(1 - \frac{E_b}{E_p}\right)} + (1 - V_f^{0.67}) E_b \tag{2}$$

The shear modulus of the particulate composite is given by a similar expression -

$$G_{pc} = \frac{V_f^{0.67} G_b}{1 - V_f^{0.33}\left(1 - \frac{G_b}{G_p}\right)} + (1 - V_f^{0.67}) G_b \tag{3}$$

Since, the constituents were assumed to have isotropic properties, the resulting composite will have isotropic properties. Therefore, the Poisson's ratio can be computed from the expression-

$$\nu_{pc} = \frac{E_{pc} - 2G_{pc}}{2G_{pc}} \tag{4}$$

Similarly, the thermal properties can be computed from analogous expressions. The coefficient of thermal expansion is given by -

$$\alpha_{pc} = \tilde{\alpha} V_f^{0.67} \frac{\tilde{E}_p}{E_{pc}} + \alpha_b \frac{E_b}{E_{pc}} - \alpha_b V_f^{0.67} \frac{E_b}{E_{pc}} \tag{5}$$

where

$$\tilde{\alpha} = \alpha_b - V_f^{0.33} (\alpha_b - \alpha_p) \tag{6}$$

and

$$\tilde{E}_p = \frac{E_b}{1 - V_f^{0.33}\left(1 - \frac{E_b}{E_p}\right)} \tag{7}$$

Similarly, the thermal conductivity of the particulate composite is given by

$$K_{pc} = \frac{V_f^{0.67} K_b}{1 - V_f^{0.33}\left(1 - \frac{K_b}{K_p}\right)} + \left(1 - V_f^{0.67}\right) K_b \tag{8}$$

and the heat capacity of the particulate composite is given by

$$C_{pc} = \frac{1}{\rho_{pc}} \left(\rho_b .(1 - V_f) C_b + \rho_p V_f C_p\right) \tag{9}$$

Similar expressions are developed for constituent microstresses and composite strength and are derived in Ref. 1. These micromechanics equations were used to predict the composite properties of Al/SiC$_p$ composite [1]. A typical result from those predictions is shown in Figure 2 comparing the prediction of composite modulus at various particle volume fractions and comparing the micromechanics predictions with other theoretical predictions as well as with mean values based on measured data [3,4]. The micromechanics predictions are well within the predicted bounds and compare very well with the measured data.

3. PROBABILISTIC SIMULATION

There are a number of approaches available for obtaining a probabilistic response from a set of independent variables and the expressions describing the response behavior. One of the most common technique is the Monte-Carlo simulation for obtaining the cumulative distribution functions (CDF's) given the probability distributions of independent variables. This technique requires a large number of simulations to generate CDF's of output variables. Although, inherently simple, the large number of output sets that must be generated to obtain a reasonably accurate CDF becomes an obvious disadvantage. NASA Glenn Research Center has been involved in developing efficient probabilistic methods for more than a decade. As a result of this research initiative, fast probability integration (FPI) algorithms were developed [2] to solve a large class of engineering problems. A brief schematic of the FPI input/output scheme is shown in Fig. 3. It is a probabilistic analysis tool that implements a variety of methods for probabilistic analysis. In general, the FPI requires the following –

1. The independent and uncorrelated input variables and their probability distributions must be defined. Constituent properties, volume fractions etc. are independent variables that in turn define a composite property, which is an output variable.
2. There must be a response function (sometimes called a performance function) that defines the relationship between the response and the independent variables.

The probability distribution of independent variables can be determined from the measured data or can be assumed on the basis of experience and judgment. The simplified micromechanics equations for the particulate composites define the response function that relate the composite properties to the input variables like constituent properties and volume fraction etc.

The uncertainties of a response variable are quantified in the form of a PDF by the following procedure:

1. The primitive variables and the corresponding probabilistic distributions are selected. (For example, to generate the PDF of the composite modulus, the particle and matrix modulus, particle volume fraction etc. could be the primitive random or independent variables).
2. For a given set of values of primitive variables, the simplified micromechanics equations for the particulate composite are used to generate the desired response variable.
3. The whole process is repeated a number of times to generate a table of response variable values that correspond to the perturbed values of the primitive variables. The number of simulations needed depends upon the method used and the number of random variables, but they are far less than what would be required in a standard Monte-Carlo technique.

4. The FPI then uses the previously generated table to compute the CDF/PDF and the corresponding sensitivities of the response.

Several methods are available in the FPI to compute a probabilistic distribution. In addition to obtaining the CDF/PDF of the response, the FPI provides additional information regarding the sensitivity of the response with respect to the primitive variables. The sensitivities provide valuable information that can be utilized to control the scatter in the response variables. The random primitive variable with the highest sensitivity factor will yield the biggest payoff in controlling the scatter in that particular response variable. Such information is very useful to the test /design engineer in designing with that material or in interpreting the experimentally measured data.

4. RESULTS/DISCUSSIONS

The material system chosen in this work was aluminum matrix reinforced with silicon carbide particles referred to as Al/SiC_p. The thermal and mechanical properties i.e. the mean values, the assumed standard deviation and the distribution types of constituent properties, and the particle volume fraction are shown in Table 1. As shown in this table, only the uncertainties in the particle volume fraction and constituent material properties are considered. The micromechanics equations were programmed in a computer code ICAN/PART (Integrated Composite Analyzer for Particulate Composites, Ref. 5). This computer code was used to generate composite properties. The FPI technique was used to obtain CDF's and probability density functions (PDF's) of the required composite properties. FPI offered very valuable additional information in the form of sensitivity factors, which represent the sensitivity of that particular output variable (composite modulus, thermal conductivity etc.) to the selected primitive random variables.

The PDF of the composite normal modulus and the corresponding sensitivity factors for a probability level of 0.5 are shown in Figs. 4 and 5. The computed mean value of composite modulus is 112.8 GPa with a standard deviation of 5.6 GPa. The scatter range of modulus (± three standard deviations) is 96 to 130 GPa. From sensitivity factors, it is clear that the composite modulus is most sensitive to matrix modulus, i.e. if one wishes to control the scatter in composite modulus, the biggest payoff could be realized by controlling the scatter in matrix modulus. Such information is very useful for test/design engineers. The sign of the sensitivity factor indicates how a specific variable influences the performance function or the scatter in the response variable under consideration. For example, a positive sensitivity value indicates a decrease in performance with an increase in the mean value of that random variable. Similar types of conclusions can be drawn from the PDF and sensitivity information for composite shear modulus shown in Figs. 6 and 7. PDF of the composite thermal expansion coefficient and the corresponding sensitivity factors at the probability level of 0.5 are shown in Figs. 8 and 9. The computed mean value is 9.49 ppm/K with a standard deviation 0.787 ppm/^{0}K. Thermal expansion coefficient of the matrix is by far the most sensitive variable followed by thermal expansion coefficient of matrix, particle volume fraction etc. The PDF of the composite thermal conductivity along with the sensitivity factors are shown in Figs. 10 and 11. Computed mean value is 141.7 W/m.^{0}C with a standard deviation of 11.3 W/m.^{0}C. Once again, thermal conductivity of the matrix is by far the most sensitive parameter followed by thermal conductivity of the silicon carbide particles and the particle volume fraction.

The sensitivity information can be utilized to reduce scatter in a desired property as mentioned earlier. As an example a separate study was conducted wherein the scatter in composite thermal expansion coefficient was targeted for improvement. The sensitivity factors of thermal expansion coefficient (Fig. 9) indicated that the thermal expansion coefficient of matrix and particles as well as particle volume fraction are most important variables, while other input parameters have little or no effect. The assumed scatter in these three most important variables was reduced by 50%. Consequently, the scatter range of composite thermal expansion coefficient was reduced as expected. The new scatter range is 8.24 to 10.74 ppm/^{0}K as shown in Fig. 12 (vs. 7.13 to 11.85 ppm/^{0}K originally). The purpose of this simulation exercise was to show that probabilistic methods can be utilized to improve the desired material properties by ranking the sensitivities and utilizing the resulting information as a guidance to appropriate quality control measures.

It is often impossible to get precise information regarding the distribution types and the nature of uncertainties in the properties of primitive variables. However, one can under those circumstances perform a series of studies experimenting with different distributions and scatter etc. As an illustration, in the present work, the effect of different probabilistic distributions of constituent properties on the composite thermal expansion coefficient is studied. Results from this study are shown in Fig. 13. The differences in the probability density functions of the composite thermal expansion coefficient appear to be minimal. The sensitivity factors (not shown) also exhibited very little difference due to different distribution types probabilistic distributions for constituent properties. In this work, distribution types for all input properties were assumed the same for that analysis - either all normal or log-normal etc. However, the technique imposes no restrictions and different distribution types for different input parameters can be given in the same analysis. If precise information about the distribution type of any input variable is not known, then these types of analyses can be performed to see their effect on the overall scatter of the response variable.

SUMMARY

A methodology that provides a formal means to quantify the scatter in particulate composite properties has been described. It takes into account the scatter in constituent properties and fabrication related parameters. The methodology combines the particulate composite micromechanics with fast probability integration technique to generate distribution functions for composite properties. Results show that the technique can provide qualitative as well as quantitative information that can be used as a guide in testing or designing with this material.

6. REFERENCES

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TABLE 1. Primitive input variables distribution parameters

VARIABLE	MEAN VALUE	STD. DEVIATION	DISTRIBUTION TYPE
Particle Volume Fraction	0.3	0.015	Normal
Young's Modulus, GPa			
SiC Particles	431.0	21.6	Normal
Al. Matrix	72.1	3.6	Normal
Poisson's Ratio			
SiC Particles	0.19	0.0095	Normal
Al Matrix	0.34	0.017	Normal
Coefficient of Thermal Expansion, 10^{-6}/K			
SiC Particles	8.6	0.86	Normal
Al Matrix	23.6	2.36	Normal
Thermal Conductivity, W/m.C			
SiC Particles	80.0	8.0	Normal
Al Matrix	178.0	17.8	Normal

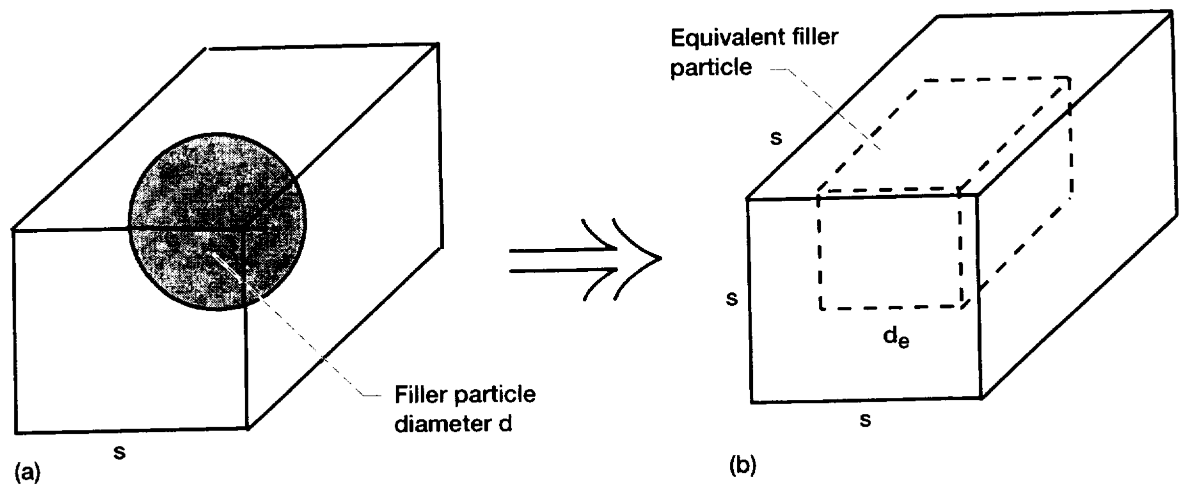

Figure 1(a).—Unit cell of the particulate composite.

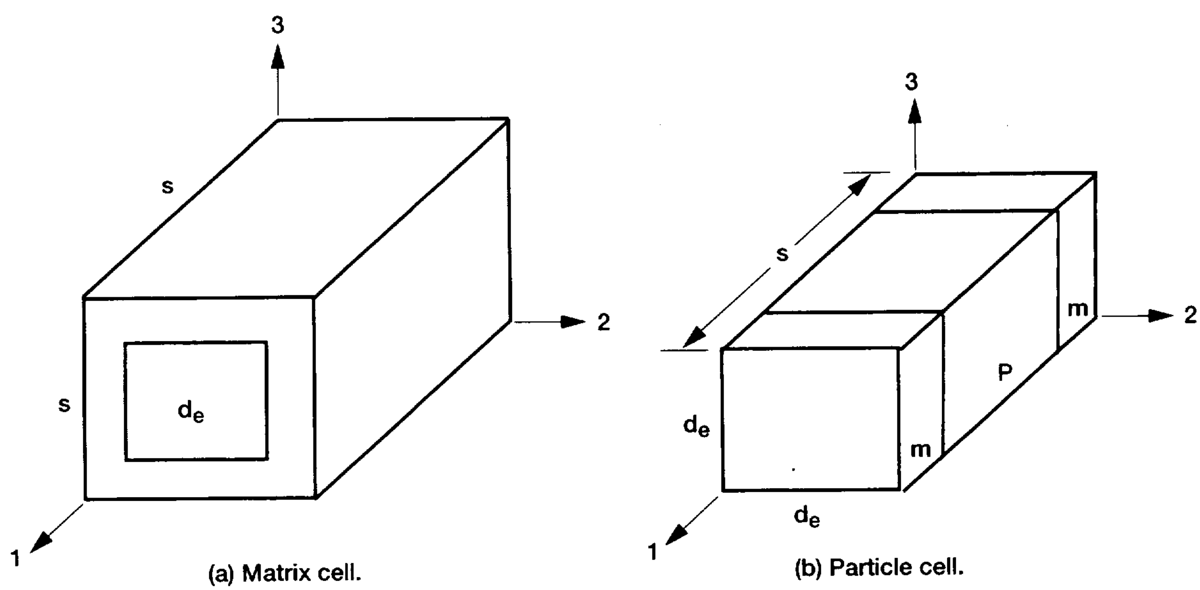

Figure 1(b).—Decomposition of unit cell-matrix (binder) and particle cells.

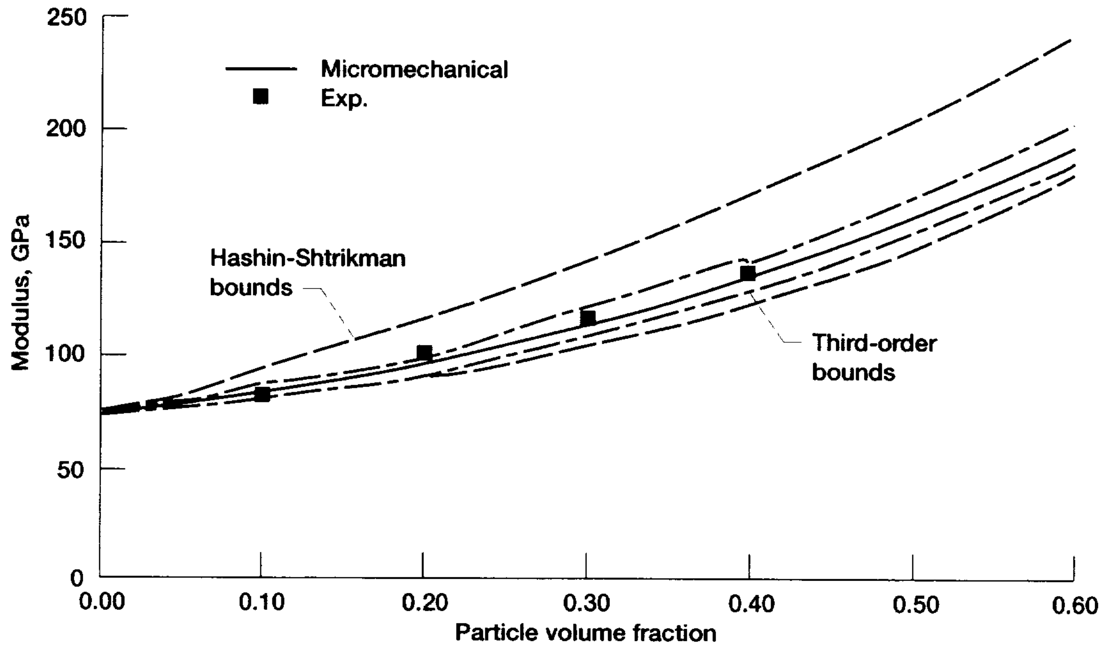

Figure 2.—Modulus of Al/SiC$_p$ composite.

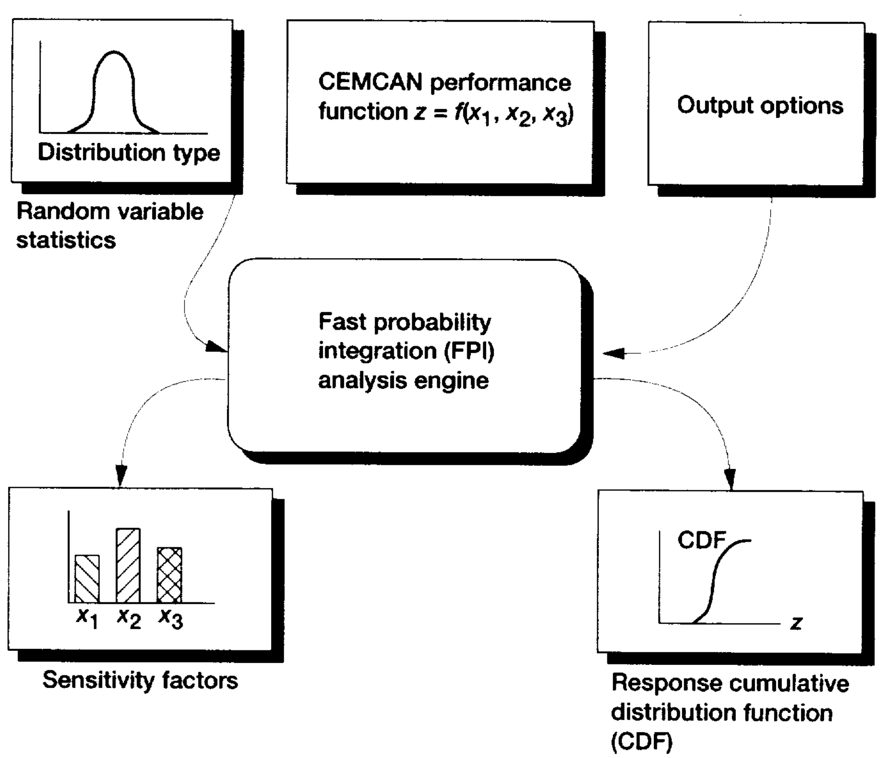

Figure 3.—Fast probability integration input-output schematic.

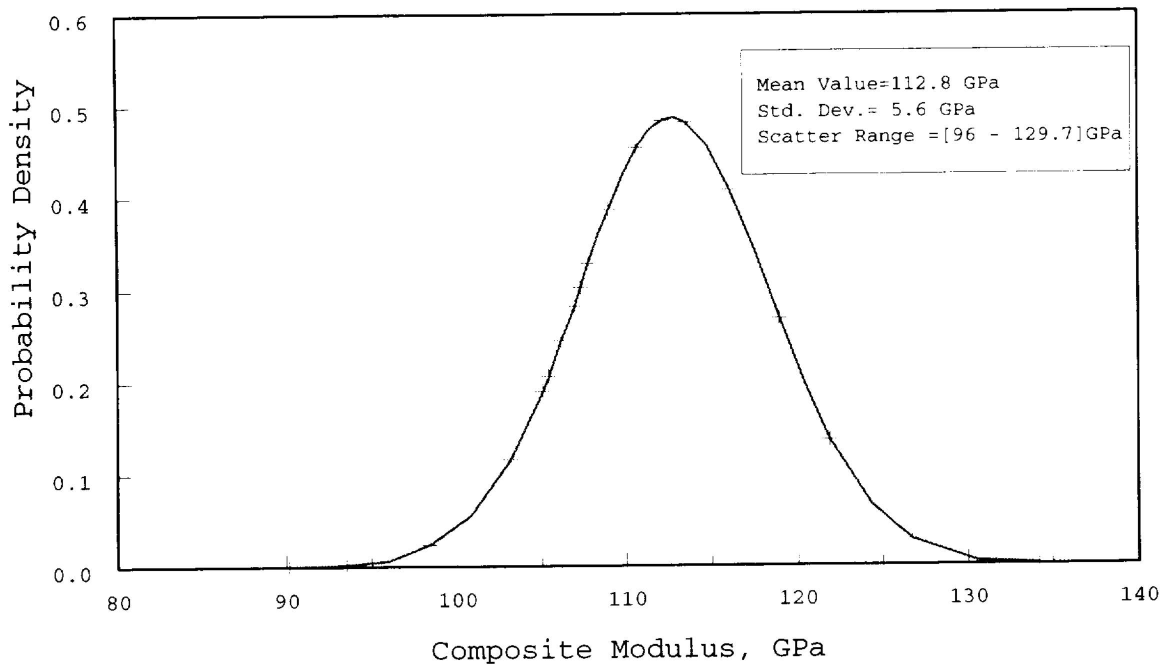

Figure 4.—Probability density function of composite Young's modulus.

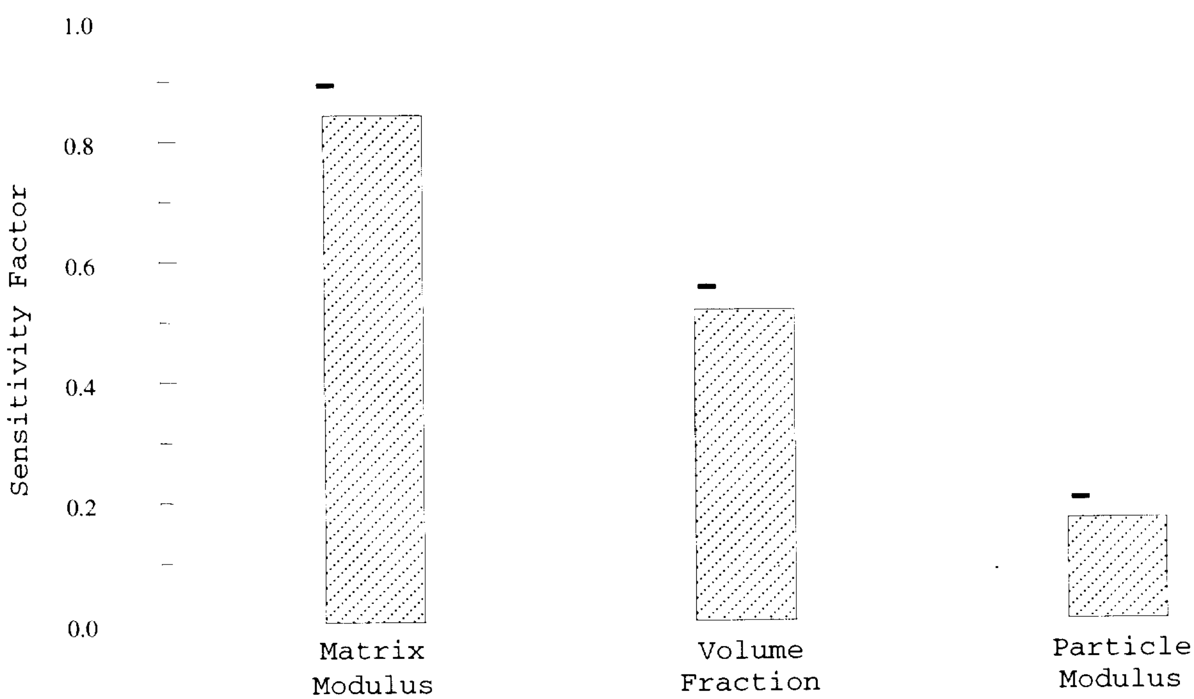

Figure 5.—Sensitivity factors of composite Young's modulus.

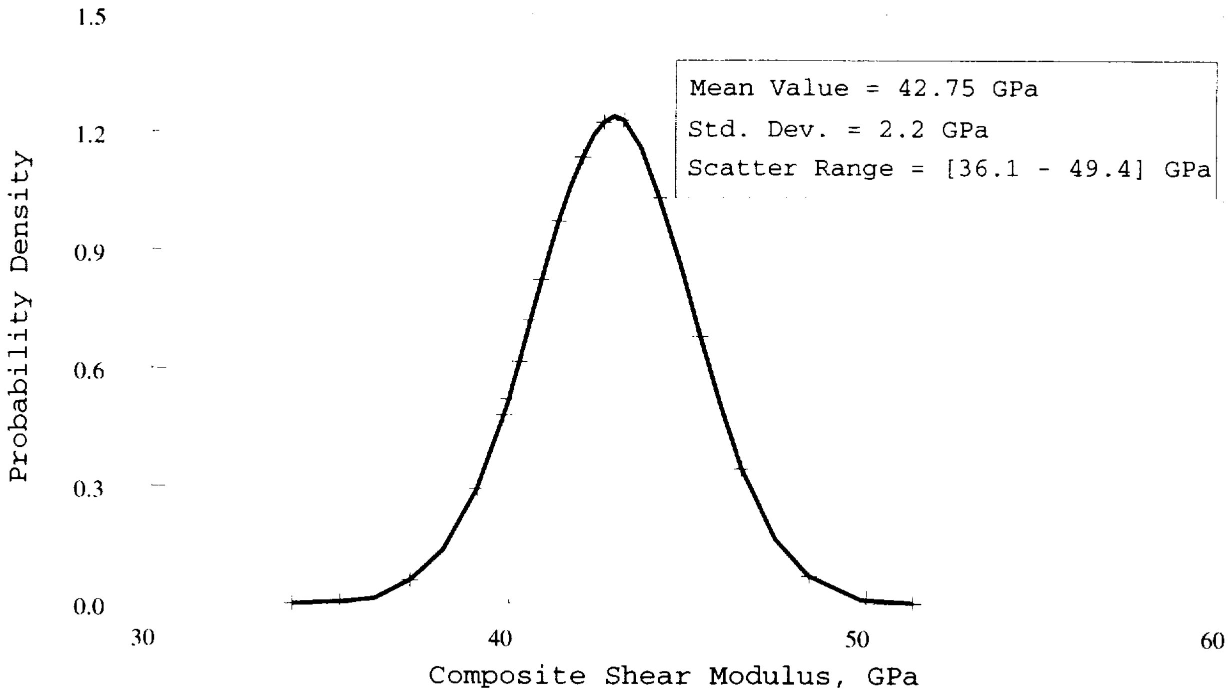

Figure 6.—Probability density function of composite shear modulus.

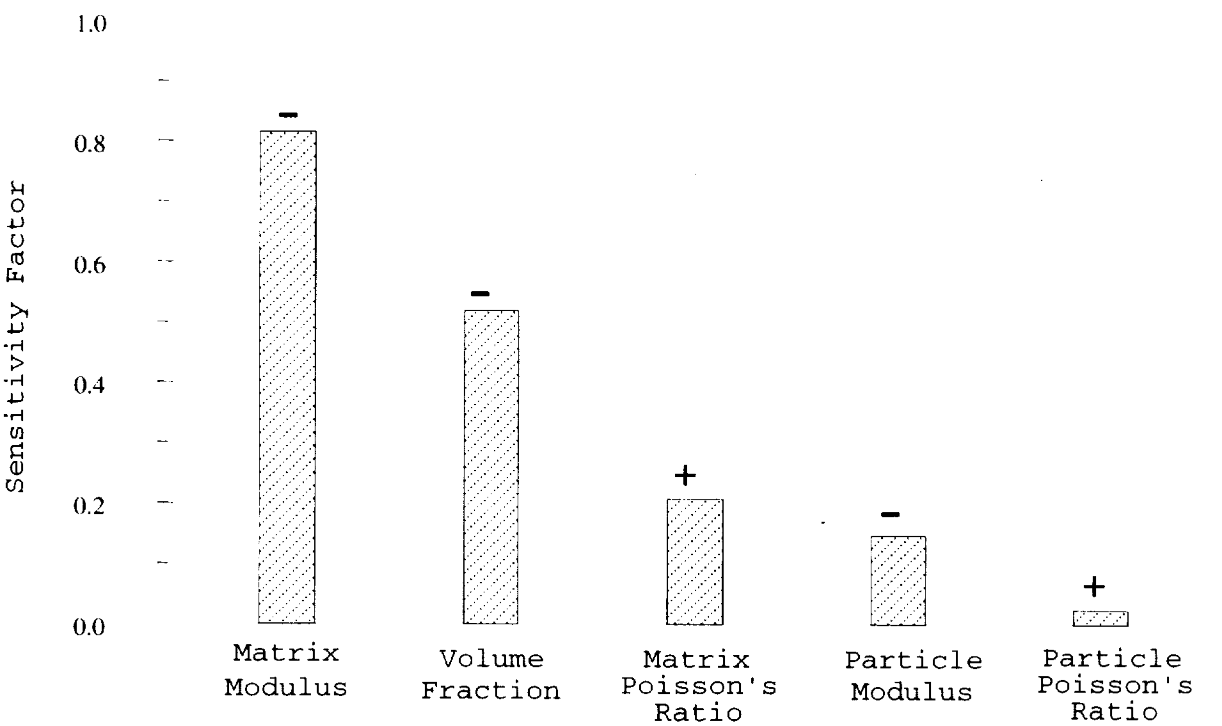

Figure 7.—Sensitivity factors of composite shear modulus.

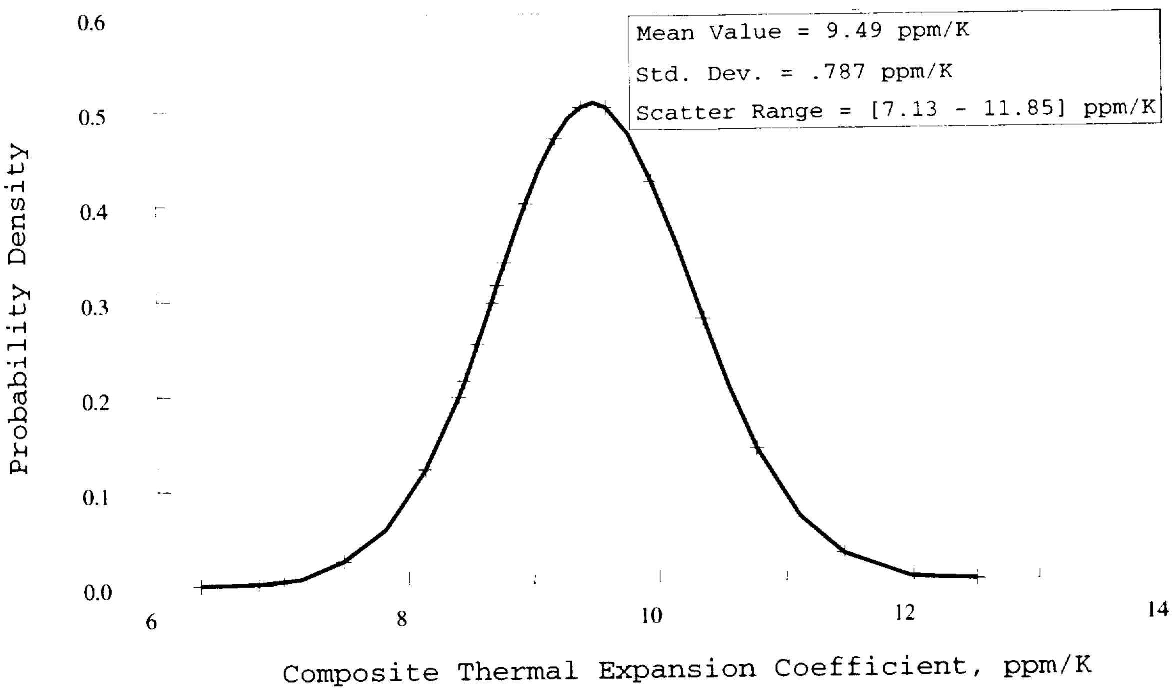

Figure 8.—Probability density function of composite thermal expansion coefficient.

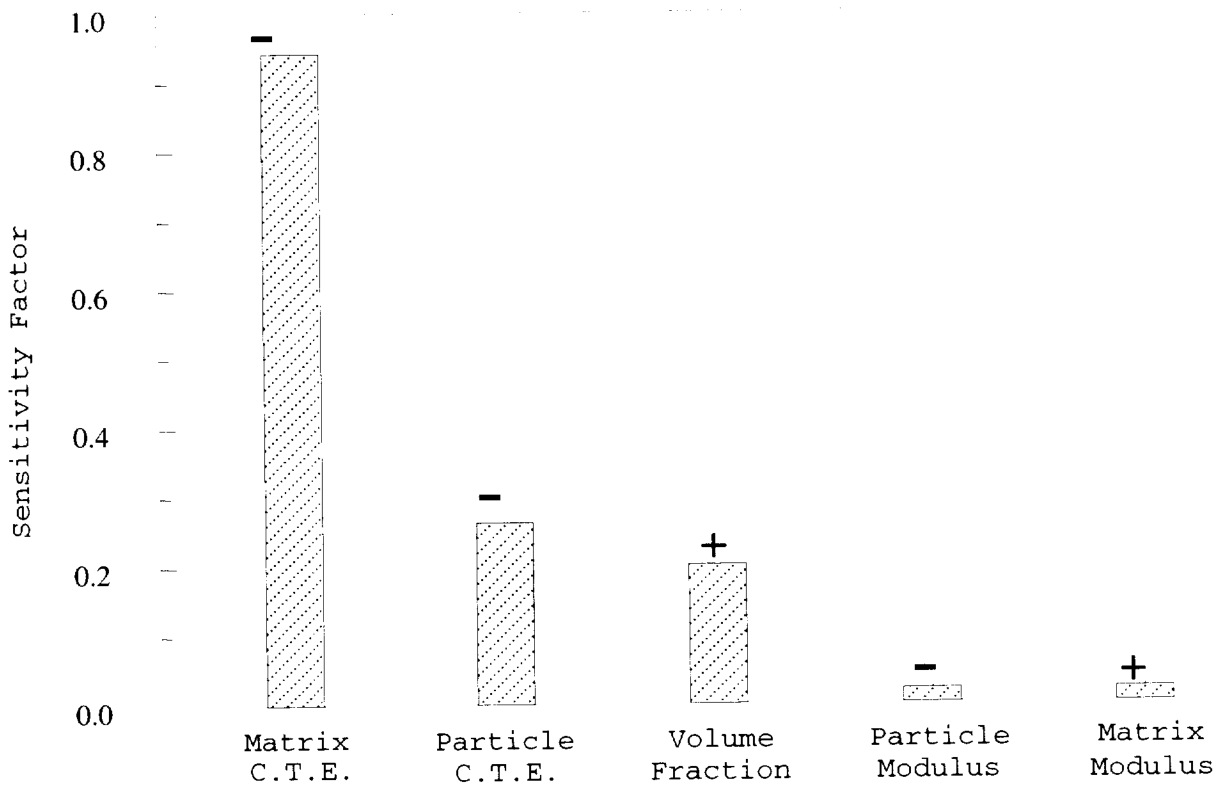

Figure 9.—Sensitivity factors of composite coefficient of thermal expansion (CTE).

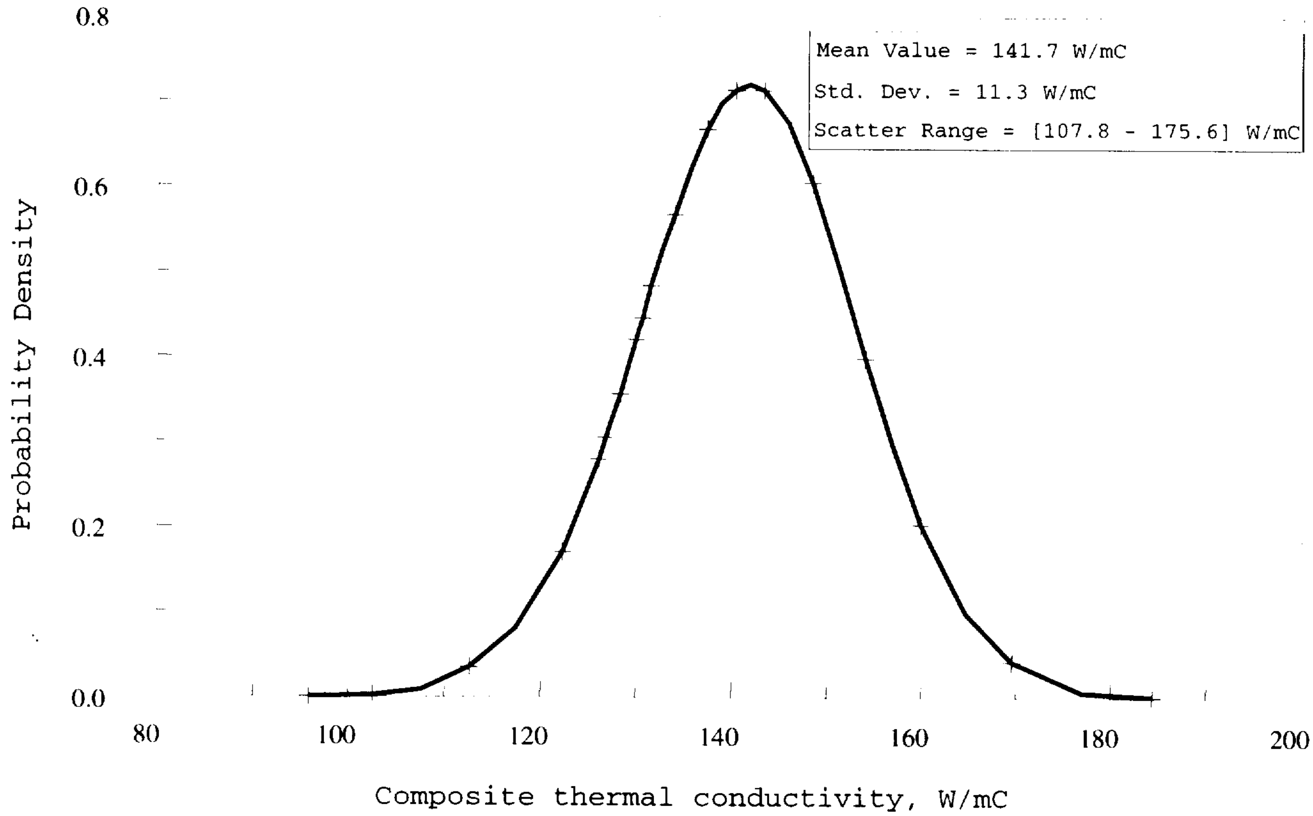

Figure 10.—Probability density function of composite thermal conductivity.

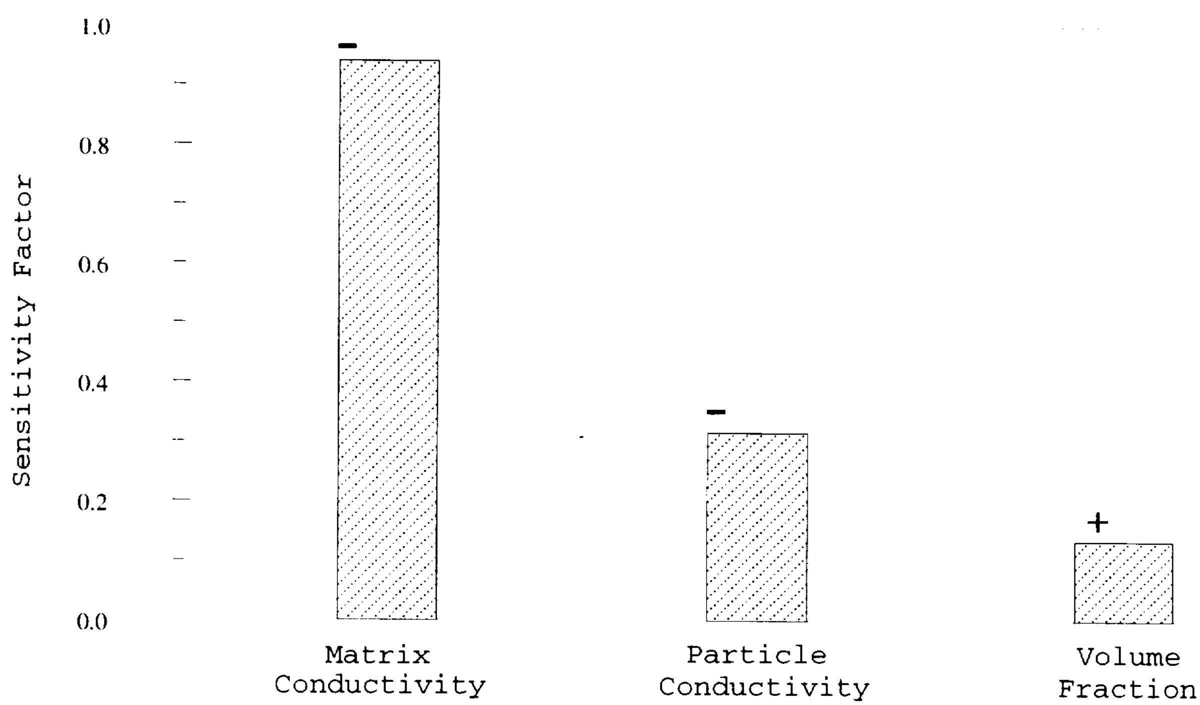

Figure 11.—Sensitivity factors of composite thermal conductivity.

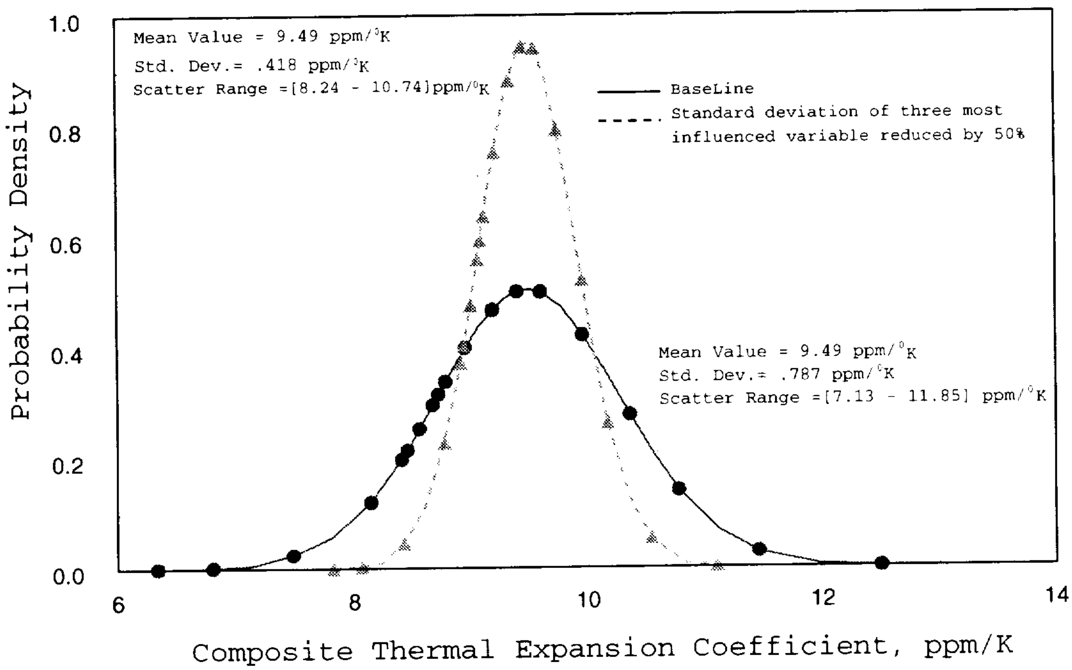

Figure 12.—Probability density function of composite thermal expansion coefficient.

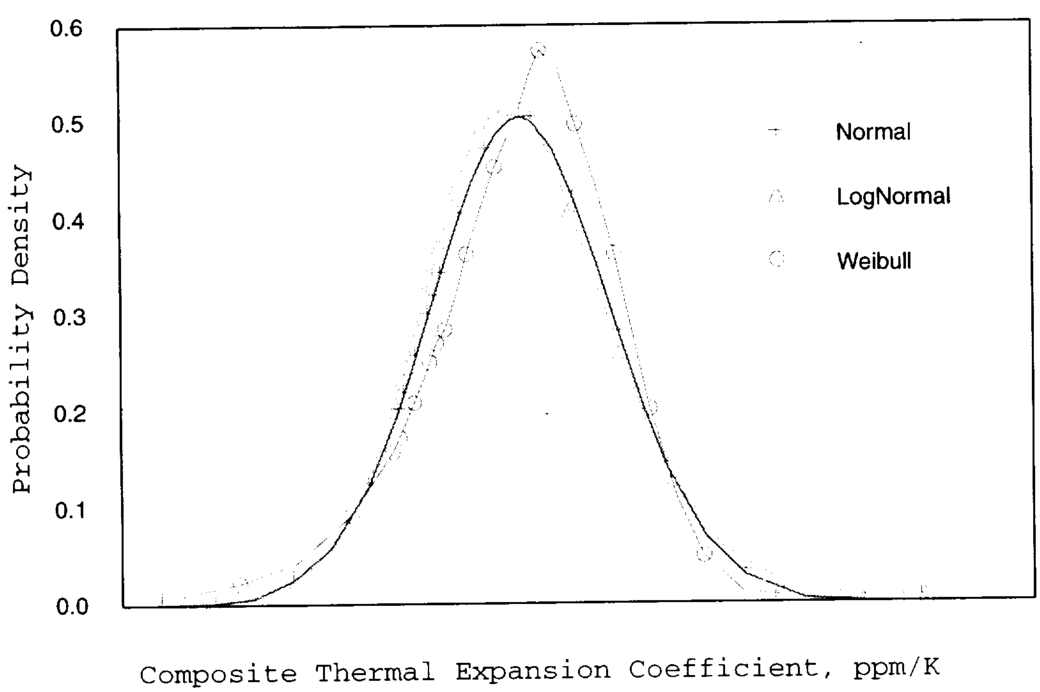

Figure 13.—Probability density function of composite thermal expansion coefficient for different distribution types for constituent properties.

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13. ABSTRACT ***(Maximum 200 words)***

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