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METal Matrix Composite ANalyzer (METCAN): Theoretical Manual

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METal Matrix Composite ANalyzer (METCAN): Theoretical Manual

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Synopsis

This manuscript is intended to be a companion volume to the "METCAN User's Manual" and the "METCAN Demonstration Manual". The primary purpose of the manual is to give details pertaining to micromechanics and macromechanics equations of high temperature metal matrix composites that are programmed in the METCAN computer code. The subroutines which contain the programmed equations are also mentioned in order to facilitate any future changes or modifications that the user may intend to incorporate in the code. Assumptions and derivations leading to the micromechanics equations are briefly mentioned.

Introduction

High temperature metal matrix composites offer great potential for use in advanced aerospace structural applications. The realization of this goal however, requires concurrent developments in (1) a technology base for fabricating high temperature metal matrix composite structural components, (2) experimental techniques for measuring thermal and mechanical characteristics, and (3) computational methods to predict their behavior. In fact, it might be argued that the development of computational methodologies should precede the others because the structural integrity and durability of high temperature metal matrix composites (HT-MMC) can be computationally simulated, and the potential payoff for a specific application can be assessed, at least qualitatively. In this way, it is possible to minimize the costly and time consuming experimental effort that would otherwise be required in the absence of a predictive capability.

Recent research into computational methods for simulating the nonlinear behavior of high temperature metal matrix composites at NASA Lewis Research Center has led to the development of the METCAN (Metal Matrix Composite ANalyzer) computer code (References 1-3). It is a computer code to simulate the high temperature nonlinear behavior of continuous fiber reinforced metal matrix composites. METCAN treats material nonlinearity at the constituent (fiber, matrix, and interphase) level, where the behavior of each constituent is modeled using a time-temperature-stress dependence. The composite properties are synthesized from the constituent instantaneous properties by making use of composite micromechanics and composite macromechanics models. Factors which affect the behavior of the composite properties include the fabrication process variables, the in-situ fiber and matrix properties, the bonding between the fiber and matrix, and/or the properties of the interphase between the fiber and matrix. The METCAN simulation is performed as point-wise analysis and produces composite properties which can be incorporated into a finite element code to perform a global structural analysis. After the global structural analysis is performed, METCAN decomposes the composite properties back into the localized response at the various levels of the simulation. At this point the constituent properties are updated and the next iteration in the analysis is initiated. This cyclic procedure is referred to as the integrated approach to metal matrix composite analysis and is depicted in Figure 1.

METCAN can be used as a stand alone code to simulate the nonlinear behavior of MMC or can be used as a module in any structural analyses package to predict the metal matrix composite structural response. It can incorporate the fabrication induced residual stresses in its simulation of composite response. A variety of physical effects such as temperature dependence, stress and stress rate dependence, fatigue due to mechanical and thermal cyclic loads can be accounted for in METCAN analysis. Furthermore, the code can be updated with relative ease to include any other physical influences that one might want to consider in a specific analysis. The documentation for the code consists of three volumes: 1) METCAN User's Manual, 2) METCAN Demonstration Manual and 3) METCAN Theoretical manual. The details of how to use the code are discussed in the first volume. The various features of METCAN and the types of analysis that METCAN can peroform are illustrated through several demonstration problems in the second volume. The theoretical manual lists all the equations pertaining to the high temperature metal matrix composites with the idea of enabling the user to update or modify the source code if necessary.

Scope

The scope of the present manual is to summarize the micromechanics equations that are programmed in the METCAN computer code. The micromechanics equations provide a basis for expressing the equivalent ply level properties of the metal matrix composite in terms of its constituent in-situ properties. Three constituents are recognized in the present code. They are the fiber, matrix and the interphase. It should be noted that the interphase can also be replaced by a compliant layer. The only difference is by virtue of the definition the interphase is a region formed between the fiber and matrix as result of a chemical reaction reducing the diameter of the fiber. A compliant layer, however, is a coating on the fiber provided intentionally to prevent such chemical reaction. Consequently, the effective fiber diameter is increased in the case of compliant layer. The mechanics involved in integrating the ply level properties to the laminate level properties (macromechanics) is well known and any text book on composites such as Reference [4] can be consulted. These details are not repeated here.

Coordinate Axes

METCAN adopts two sets of cartesian coordinate axes for presenting the results. They are the material axes and the structural axes as shown in Figure 2. The material axes are defined with respect to fiber orientation. The direction along the fiber is denoted as 1-1 or 11 and the directions transverse to the fiber are denoted 2-2 (22) and 3-3 (33) respectively. All the ply level properties and responses are expressed with respect to the material axes system. The global/laminate level properties and responses are given in the structural axes system. They are denoted by x, y, and z. Any quantity with a normal orientation is represented by the subscripts xx, yy, and zz. The shear orientations are indicated by subscripts xy, yz, and zx.. Also, the coordinate axes definitions are printed as a part of the output for easier interpretation.

Units

The primary units chosen in METCAN are the British system of units. All of the constituent properties in the resident data bank are expressed accordingly: inches (for length), pounds (for forces), degrees Fahrenheit (for temperatures), BTU's for heat, seconds/hours (for time) and psi/ksi/Mpsi (for stress and stiffness related quantities). A table of units (Table 1) is provided (by default as one of the output options) at the beginning of the METCAN output for easy reference. Any user wishing to employ another system of units may do so by updating the data bank properties into the preferred system. The output will then reflect the appropriate unit system chosen by the user. Nevertheless, the user should exercise some caution as there may have been some hard wired conversions of units within the source code (e. g. conversions of psi to ksi, or mpsi are done by dividing with 1000 or 1000000 with in the code in order to print some of the variables in the most appropriate and concise format)

Glossary of symbols

11, 22, 33	subscripts for longitudinal and transverse directions in the material coordinate system
f, m, d, and l	subscripts for fiber, matrix, interphase and ply
A, B, C	unit cell subregions
C	heat capacity
E	Young's modulus
D	Current diameter of the fiber
D_o	Outer diameter of the fiber
G	Shear modulus
K	thermal conductivity
T	temperature
0	suffix for the reference (room temp.) quantities
k	fiber volume ratio
α	thermal expansion coefficient
ν	Poisson's ratio
σ	stress
ρ	density
ΔT	temperature differential

Nonlinear Material Behavior Models

METCAN treats material nonlinearity at the constituent level through the incorporation of a multifactor interaction relationship (MFIR). The MFIR models the material behavior in the form of a time-temperature-stress dependence of the constituent properties. The MFIR and the rationale for its utilization are expressed in Figure 3. The form of the MFIR is a product function of terms raised to specified powers that define the values of the material property (P) of the fiber, matrix, and interphase. The constituent properties (P) which are determined through the MFIR are modulus, Poisson's ratio, strength, coefficient of thermal expansion, thermal conductivities. The density and heat capacity are considered as constants. For each fiber, matrix and interphase property, there is generally a distinct set of values of the exponents necessary to express the functional definition of the property. The various exponents are determined from the appropriate experimental data. The variation of a typical property as a function of one such factor is shown in Figure 4 for various exponent values. As seen from the figure, one can nullify any of the physical effects (e. g. temperature dependence) by simply choosing a "zero" exponent. A linear variation can be achieved by taking a value of "one" for the exponent. The property value must be matched carefully at the reference point and at the final point from the appropriate experimental data. The actual nonlinear behavior between these two points is dependent on the value of the exponent which is usually of a second order effect.

The coding for the material behavior modeling is done through a set of six subroutines in the METCAN code. The thermal properties are updated in the subroutines THERF, THERM, and THERD respectively for fiber, matrix and interphase properties. The mechanical properties are updated in the subroutines MECF, MECM, and MECD respectively for fiber, matrix and interphase properties.

METCAN unit cell

In METCAN the global behavior is obtained by successive integration of the response/properties from the constituent level to laminate level using micromechanics and macromechanics. The micromechanics embedded in METCAN is based upon the usual assumptions pertaining to the mechanics of materials approach [Ref. 4-5]. The derivation of equivalent composite properties using micromechanics theory starts with the identification of a representative volume element or unit cell. It is the smallest region or piece of material over which the stresses and strains are macroscopically uniform. However, within the unit cell the stresses and strains are nonuniform due to the heterogeneity of the material. It is assumed that these cells are arranged in a regular square array pattern. The principal assumptions involved in the mechanics of materials approach are (1) fiber and matrix are subjected to the same strain in the fiber direction of a unidirectional fibrous composite and (2) the same transverse stress is applied to both the fiber and matrix in the direction transverse to the fiber. The details of the representative volume element chosen in the development METCAN is shown in Figure 5. The unit cell for METCAN consists of a maximum of three regions, A, B, and C. The region A consists of matrix only, the region B consists of a combination of matrix and interphase, and the region C consists of a combination of all three constituents: fiber, matrix and interphase. Note, that in the following discussion the interphase is treated as a separate constituent with distinct properties. Thus, it can either represent a zone formed due to a chemical reaction between the fiber and matrix or a separate layer provided intentionally to prevent such a reaction. In the figure 5 D represents the current diameter of the fiber and D_o represents the outer diameter. The outer diameter is either the undamaged fiber diameter if there is an interphase or the diameter of the fiber with the compliant layer coating if there is a compliant layer. The different regions A, B, and C of unit cell facilitate the representation of nonuniformity in the local stress distribution.

Microstresses in Regions A, B, and C of METCAN unit cell

The properties of the constituents forming the unit cell in the regions A, B, and C are updated incrementally at the end of each iteration depending upon the local response (stress, stress rate, temperature etc..). The local response is obtained by progressively decomposing the global response to ply response (ply stresses) and applying the micromechanics at the unit cell. The stresses in the various regions of unit cell are termed as "microstresses" in METCAN. These calculations are performed in the METCAN microstress calculation module which consists of a set of four subroutines STRESF, STRESM, STRESD and STRESI. The first three pertain to the calculation of microstresses in the various regions for fiber, matrix and interphase respectively. Operations common to these three are grouped together into a common subroutine STRESI which is called before calling the rest of the three subroutines. The following few paragraphs lists the various equations that are currently programmed in METCAN to perform the microstress calculations.

Stresses due to temperature differences

The following equations show how microstresses due to temperature differences in the fiber, microstresses in matrix in regions A, B and C, and microstresses in interphase in regions B and C are calculated in METCAN. It should be noted that temperature differences cause microstressess due to two reasons. The first one is due to differences in constituents thermal expansion coefficients. The second one is due to the ply stresses that are developed as a result of different ply orientations. The latter is described in the next section "stresses due to mechanical loads".

Microstresses along the longitudinal (11) direction:

Fiber Microstresses: The fiber longitudinal microstress due to a uniform temperature difference ΔT can be given by

$$\sigma_{f11} = \{\alpha_{l11} - \alpha_{f11}\} E_{f11} \Delta T \tag{1}$$

In the above equation the longitudinal stress in fiber due to a temperature difference is calculated using the differential expansion between the fiber and ply. However, in METCAN it is calculated from the stress equilibrium along the fiber direction using the following equation.

$$\sigma_{f11} = -\left[\left\{\left(\frac{D_0}{D}\right)^2 - 1\right\}\sigma_{d11} + \left(\frac{D_0}{D}\right)^2 \sigma_{m11}\left(\frac{1-k_f}{k_f}\right)\right] \tag{2}$$

The above equation forces fiber stress to be in equilibrium with those of matrix and interphase.

Matrix Microstresses: The matrix microstress has two components σ_{m11T} and σ_{m11NU} where the part of the subscript T and NU denote the normal and Poisson's contributions respectively. They are given by

$$\sigma_{m11T} = \{\alpha_{l11} - \alpha_{m11}\} E_{m11} \Delta T \tag{3}$$

$$\sigma_{m11NU} = \Big[\ 1/6\ \Big\{ \nu_{m21A}\left(\alpha_{l22} - \alpha^{A}_{m22}\right) + \nu_{m21B}\left(\alpha_{l22} - \alpha^{B}_{m22}\right) + \nu_{m21C}\left(\alpha_{l22} - \alpha^{C}_{m22}\right) + \nu_{m31A}\left(\alpha_{l22} - \alpha^{A}_{m33}\right) + \nu_{m31B}\left(\alpha_{l22} - \alpha^{B}_{m33}\right) + \nu_{m31C}\left(\alpha_{l22} - \alpha^{B}_{m33}\right) \Big\}\ \Big] E_{m11} \Delta T \tag{4}$$

$$\sigma_{m11} = \sigma_{m11T} + \sigma_{m11NU} \tag{5}$$

Interphase Microstresses: The interphase microstress, similarly, has two components σ_{d11T} and σ_{d11NU} which are given by

$$\sigma_{d11T} = \left\{\alpha_{l11} - \alpha^{B}_{d11}\right\} E_{d11} \Delta T \tag{6}$$

$$\sigma_{d11NU} = \Big[\ 1/4 \Big\{ \nu_{d21B}(\alpha_{l22} - \alpha^{B}_{d22}) + \nu_{d21C}(\alpha_{l22} - \alpha^{C}_{d22}) + \nu_{d31B}(\alpha_{l22} - \alpha^{B}_{d33}) + \nu_{d31A}(\alpha_{l22} - \alpha^{C}_{d33}) \Big\}\ \Big] E_{d11} \Delta T \tag{7}$$

$$\sigma_{d11} = \sigma_{d11T} + \sigma_{d11NU} \tag{8}$$

<u>Microstresses along the transverse (22 and 33) directions:</u>

Transverse fiber microstresses:

$$\sigma_{f22C} = \sigma_{m22C} \qquad \sigma_{f33C} = \sigma_{m33C} \tag{9}$$

Note that in the above it is assumed that both the fiber and matrix develop the same microstress in 22 and 33 directions.

Transverse (22 &33) thermal microstresses in matrix Region A: The tranverse thermal microstresses due to a temperature differential ΔT is computed by considering the differential expansion of the region A and the ply. The end result is

$$\sigma_{m22A} = \left\{\alpha_{l22} - \alpha_{m22A} + \nu_{m12A}(\alpha_{l11} - \alpha_{m11}) + \nu_{m32A}(\alpha_{l33} - \alpha_{m33A})\right\} \Delta T E_{m22A} \tag{10}$$

$$\sigma_{m33A} = \left\{\alpha_{l33} - \alpha_{m33A} + \nu_{m13A}(\alpha_{l11} - \alpha_{m11}) + \nu_{m23A}(\alpha_{l22} - \alpha_{m22A})\right\} \Delta T E_{m33A} \tag{11}$$

Transverse (22 & 33) thermal microstresses in matrix Region B: These microstresses are derived along the same lines as the above. However, since the region B consists of both matrix and interphase, there are contributions from both constituents. Furthermore, both interphase and matrix will have the same stress given by the following equations:

$$\sigma_{m22B} = \left[-\frac{\sqrt{k_f}}{(1-\sqrt{k_f})} \nu_{d12B}\{\alpha_{l11}-\alpha_{d11}\} - \nu_{m12B}\{\alpha_{l11}-\alpha_{m11}\} \right. - \frac{\sqrt{k_f}}{(1-\sqrt{k_f})} \nu_{d32B}\{\alpha_{l33}-\alpha_{d33B}\} - \nu_{m32B}\{\alpha_{l33}-\alpha_{m33B}\} \left. + \frac{\alpha_{l22}}{(1-\sqrt{k_f})} - \frac{\sqrt{k_f}}{(1-\sqrt{k_f})} \alpha_{d22B} - \alpha_{m22B} \right] \frac{\Delta T(1-\sqrt{k_f})E_{d22B}}{\left\{ \sqrt{k_f} + (1-\sqrt{k_f}) \dfrac{E_{d22B}}{E_{m22B}} \right\}} \tag{12}$$

$$\sigma_{m33B} = \left[-\frac{\sqrt{k_f}}{(1-\sqrt{k_f})} \nu_{d13B}\{\alpha_{l11}-\alpha_{d11}\} - \nu_{m13A}\{\alpha_{l11}-\alpha_{m11}\} \right. - \frac{\sqrt{k_f}}{(1-\sqrt{k_f})} \nu_{d23B}\{\alpha_{l22}-\alpha_{d22B}\} - \nu_{m23B}\{\alpha_{l22}-\alpha_{m22B}\} \left. + \frac{\alpha_{l33}}{(1-\sqrt{k_f})} - \frac{\sqrt{k_f}}{(1-\sqrt{k_f})} \alpha_{d33B} - \alpha_{m33B} \right] \frac{\Delta T(1-\sqrt{k_f})E_{d33B}}{\left\{ \sqrt{k_f} + (1-\sqrt{k_f}) \dfrac{E_{d33B}}{E_{m33B}} \right\}} \tag{13}$$

Transverse (22 & 33) thermal microstress in matrix region C: These are calculated by forcing the equilibrium in the respective directions. The following are the appropriate equations:

$$\sigma_{m22C} = -\frac{(1-\sqrt{k_f}\,)}{\sqrt{k_f}} \frac{D_0}{D} \sigma_{m22A} - \left\{1-\frac{D}{D_0}\right\} \frac{D_0}{D} \sigma_{m22B} \tag{14}$$

$$\sigma_{m33C} = -\frac{(1-\sqrt{k_f}\,)}{\sqrt{k_f}} \frac{D_0}{D} \sigma_{m33A} - \left\{1-\frac{D}{D_0}\right\} \frac{D_0}{D} \sigma_{m33B} \tag{15}$$

Transverse microstressess in the interphase regions B and C: These are assumed to be same as those for the matrix regions B and C.

$$\begin{aligned} \sigma_{d22B} &= \sigma_{m22B} \\ \sigma_{d33B} &= \sigma_{m33B} \\ \sigma_{d22C} &= \sigma_{m22C} \\ \sigma_{d33C} &= \sigma_{m33C} \end{aligned} \tag{16}$$

This completes the summary of equations for microstresses due to temperature differential.

Stresses due to mechanical loads

The mechanical loads applied globally are progressively decomposed using macromechanics/laminate theory to ply stresses and these stresses are passed on to the microstresses calculation module. It should be noted that, eventhough they are treated as mechanical loads, contributions arising due to thermal loads are included in the ply stresses. The ply stresses are assumed to have been applied to the unit cell. The constituent microstress contribution corresponding to each of the these ply stresses in each of the regions A, B and C are calculated using the mechanics of materials approach.

Fiber Microstresses due to applied ply normal stresses

Stresses along the longitudinal (11) direction: The fiber longitudinal (11) stresses due to the three normal applied ply stresses are given by

$$\begin{aligned}
\sigma_{f11}^{(1)} &= E_{f11}\,\frac{\sigma_{l11}}{E_{l11}} \\
\sigma_{f11}^{(2)} &= -\,(\nu_{l21}-\nu_{f21})\frac{E_{f11}}{E_{l22}}\sigma_{l22} \\
\sigma_{f11}^{(3)} &= -\,(\nu_{l31}-\nu_{f31})\frac{E_{f11}}{E_{l33}}\sigma_{l33} \\
\sigma_{f11} &= \sigma_{f11}^{(1)} + \sigma_{f11}^{(2)} + \sigma_{f11}^{(3)}
\end{aligned} \tag{17}$$

Note that in the above the superscripts $^{(1)}$, $^{(2)}$, and $^{(3)}$ represents the contributions to a specific microstress due to the applied ply stress in 11, 22 and 33 directions respectively.

Stresses along the transverse (22) direction: The fiber transverse (22) microstress due to the three normal applied ply stresses are given by

$$\sigma_{f22}^{(2)} = E_{22C}\,\frac{\sigma_{l22}}{E_{l22}} \tag{18}$$

$$\sigma_{f22}^{(1)} = -\left[\nu_{l12}-(1-\sqrt{k_f})\,\nu_{m12C}-\sqrt{k_f}\left(\left\{1-\frac{D_0}{D}\right\}\nu_{d12C}+\frac{D}{D_0}\nu_{f12}\right)\right]\frac{\sigma_{l11}}{E_{l11}}\,E_{22C} \tag{19}$$

$$\sigma_{f22}^{(3)} = -\left[\nu_{l32}-(1-\sqrt{k_f})\,\nu_{m32C}-\sqrt{k_f}\left(\left\{1-\frac{D_0}{D}\right\}\nu_{d32C}+\frac{D}{D_0}\nu_{f32}\right)\right]\frac{\sigma_{l33}}{E_{l33}}\,E_{22C} \tag{20}$$

In the above the E_{22C} is given by

$$E_{22C} = \frac{1}{\left[\frac{(1-\sqrt{k_f})}{E_{m22C}} + \frac{\sqrt{k_f}}{E_{d22C}}\left\{1-\frac{D}{D_0}\right\} + \frac{\sqrt{k_f}}{E_{f22}}\frac{D}{D_0}\right]} \tag{21}$$

$$\sigma_{f22} = \sigma_{f22}^{(1)} + \sigma_{f22}^{(2)} + \sigma_{f22}^{(3)} \tag{22}$$

Stresses along the transverse (33) direction: These are analogous to the 2-2 direction stresses and are given by

$$\sigma_{f33}^{(3)} = E_{33C}\frac{\sigma_{l33}}{E_{l33}} \tag{23}$$

$$\sigma_{f33}^{(1)} = -\left[\nu_{l13}-(1-\sqrt{k_f})\,\nu_{m13C}-\sqrt{k_f}\left(\left\{1-\frac{D_0}{D}\right\}\nu_{d13C} + \frac{D}{D_0}\nu_{f13}\right)\right]\frac{\sigma_{l11}}{E_{l11}}E_{33C} \tag{24}$$

$$\sigma_{f33}^{(2)} = -\left[\nu_{l23}-(1-\sqrt{k_f})\,\nu_{m23C}-\sqrt{k_f}\left(\left\{1-\frac{D_0}{D}\right\}\nu_{d23C} + \frac{D}{D_0}\nu_{f22}\right)\right]\frac{\sigma_{l22}}{E_{l22}}E_{33C} \tag{25}$$

In the above the E_{33C} is given by

$$E_{33C} = \frac{1}{\left[\frac{(1-\sqrt{k_f})}{E_{m33C}} + \frac{\sqrt{k_f}}{E_{d33C}}\left\{1-\frac{D}{D_0}\right\} + \frac{\sqrt{k_f}}{E_{f33}}\frac{D}{D_0}\right]} \tag{26}$$

$$\sigma_{f33} = \sigma_{f33}^{(1)} + \sigma_{f33}^{(2)} + \sigma_{f33}^{(3)} \tag{27}$$

Matrix microstresses due to applied ply normal stresses

Stresses along the longitudinal (11) direction in region A: The matrix longitudinal stresses due to the three normal applied ply stresses are given by

$$\begin{aligned}
\sigma_{m11A}^{(1)} &= E_{m11A}\frac{\sigma_{l11}}{E_{l11}} \\
\sigma_{m11A}^{(2)} &= (\nu_{l21}-\nu_{f21})\frac{E_{f11}}{E_{l22}}\sigma_{l22}\frac{k_f}{(1-k_f)} \\
\sigma_{m11A}^{(3)} &= (\nu_{l31}-\nu_{f31})\frac{E_{f11}}{E_{l33}}\sigma_{l33}\frac{k_f}{(1-k_f)}
\end{aligned} \tag{28}$$

Stresses along the longitudinal (11) direction in regions B and C: These are given by similar expressions as above. However, the Poisson's contributions (the second and the third of the above equations 28) are taken as same as above.

$$\sigma_{m11B}^{(1)} = E_{m11B}\frac{\sigma_{l11}}{E_{l11}} \qquad \sigma_{m11C}^{(1)} = E_{m11C}\frac{\sigma_{l11}}{E_{l11}} \tag{29}$$

The total matrix microstress is given by adding each contribution.

$$\begin{aligned}\sigma_{m11A} &= \sigma_{m11A}^{(1)} + \sigma_{m11A}^{(2)} + \sigma_{m11A}^{(3)}\\ \sigma_{m11B} &= \sigma_{m11B}^{(1)} + \sigma_{m11B}^{(2)} + \sigma_{m11B}^{(3)}\\ \sigma_{m11C} &= \sigma_{m11C}^{(1)} + \sigma_{m11C}^{(2)} + \sigma_{m11C}^{(3)}\end{aligned} \tag{30}$$

Stresses along the transverse (22) direction in regions A, B, and C: The transverse microstresses in the matrix region B and C are calculated first and the region A microstress is obtained by forcing equilibrium in 22 direction. The microstresses in region B due to the three normal applied ply stresses are given by

$$\begin{aligned}\sigma_{m22B}^{(2)} &= \sigma_{l22}\frac{E_{22B}}{E_{l22}}\\ \sigma_{m22B}^{(1)} &= -\frac{\sigma_{l11}E_{22B}}{E_{l11}}\left\{\nu_{l12}-\nu_{m12B}(1-\sqrt{k_f})-\sqrt{k_f}\nu_{d12B}\right\}\\ \sigma_{m22B}^{(3)} &= -\frac{\sigma_{l33}E_{22B}}{E_{l33}}\left\{\nu_{l32}-\nu_{m32B}(1-\sqrt{k_f})-\sqrt{k_f}\nu_{d32B}\right\}\\ E_{22B} &= \frac{E_{d22B}}{\left(\sqrt{k_f} + (1-\sqrt{k_f})\,\dfrac{E_{d22B}}{E_{m22B}}\right)}\end{aligned} \tag{31}$$

By adding the above three contributions the total microstress in region B is obtained as

$$\sigma_{m22B} = \sigma_{m22B}^{(1)} + \sigma_{m22B}^{(2)} + \sigma_{m22B}^{(3)} \tag{32}$$

The region C stresses in matrix, similarly, can be expressed by the following set of equations

$$\sigma^{(2)}_{m22C} = \sigma_{l22}\frac{E_{22C}}{E_{l22}}$$

$$\sigma^{(1)}_{m22C} = \frac{\sigma_{l11}E_{22C}}{E_{l11}}\left\{\nu_{l12}-\nu_{m12C}(1-\sqrt{k_f})-\sqrt{k_f}\left(\nu_{d12C}\left\{1-\frac{D}{D_0}\right\}+\frac{D}{D_0}\nu_{f12}\right)\right\} \tag{33}$$

$$\sigma^{(3)}_{m22C} = \frac{\sigma_{l33}E_{22C}}{E_{l33}}\left\{\nu_{l32}-\nu_{m32B}(1-\sqrt{k_f})-\sqrt{k_f}\left(\nu_{d32C}\left\{1-\frac{D}{D_0}\right\}+\frac{D}{D_0}\nu_{f32}\right)\right\}$$

where E_{22C} is given by equation (21).
By adding the above three contributions the total microstress in region B is obtained as

$$\sigma_{m22C} = \sigma^{(1)}_{m22C} + \sigma^{(2)}_{m22C} + \sigma^{(3)}_{m22C} \tag{34}$$

The Region A stresses are given by

$$\sigma^{(2)}_{m22A} = \sigma_{l22}\frac{E_{m22A}}{E_{l22}}$$

$$\sigma^{(1)}_{m22A} = -\sqrt{k_f}\left[\left\{1-\frac{D}{D_0}\right\}\sigma^{(1)}_{m22B} + \frac{D}{D_0}\sigma^{(1)}_{m22C}\right] \tag{35}$$

$$\sigma^{(3)}_{m22A} = -\sqrt{k_f}\left[\left\{1-\frac{D}{D_0}\right\}\sigma^{(3)}_{m22B} + \frac{D}{D_0}\sigma^{(3)}_{m22C}\right]$$

$$\sigma_{m22A} = \sigma^{(1)}_{m22A} + \sigma^{(2)}_{m22A} + \sigma^{(3)}_{m22A}$$

Stresses along the 33 direction in Regions A, B, and C: The microstresses in 3-3 direction are given by analogous expressions as those for the 2-2 directions and may be obtained by appropriately changing the subscripts 22 to 33. For the sake of completeness they are given below:

$$
\begin{aligned}
\sigma^{(2)}_{m33B} &= \sigma_{l33}\frac{E_{33B}}{E_{l33}} \\
\sigma^{(1)}_{m33B} &= \frac{\sigma_{l11}E_{33B}}{E_{l11}}\left\{\nu_{l13}-\nu_{m13B}(1-\sqrt{k_f})-\sqrt{k_f}\nu_{d13B}\right\} \\
\sigma^{(2)}_{m33B} &= \frac{\sigma_{l22}E_{33B}}{E_{l22}}\left\{\nu_{l23}-\nu_{m23B}(1-\sqrt{k_f})-\sqrt{k_f}\nu_{d23B}\right\} \\
E_{33B} &= \frac{E_{d33B}}{\left(\sqrt{k_f} + (1-\sqrt{k_f})\,\frac{E_{d33B}}{E_{m33B}}\right)}
\end{aligned}
\tag{36}
$$

By adding the above three contributions the total microstress in region B is obtained as

$$
\sigma_{m33B} = \sigma^{(1)}_{m33B} + \sigma^{(2)}_{m33B} + \sigma^{(3)}_{m33B} \tag{37}
$$

The region C stresses in matrix, similarly, can be expressed by the following set of equations

$$
\begin{aligned}
\sigma^{(2)}_{m33C} &= \sigma_{l33}\frac{E_{33C}}{E_{l33}} \\
\sigma^{(1)}_{m33C} &= \frac{\sigma_{l11}E_{33C}}{E_{l11}}\left\{\nu_{l13}-\nu_{m13C}(1-\sqrt{k_f})-\sqrt{k_f}\left(\nu_{d13C}\left\{1-\frac{D}{D_0}\right\}+\frac{D}{D_0}\nu_{f13}\right)\right\} \\
\sigma^{(2)}_{m33C} &= \frac{\sigma_{l22}E_{33C}}{E_{l22}}\left\{\nu_{l23}-\nu_{m23B}(1-\sqrt{k_f})-\sqrt{k_f}\left(\nu_{d23C}\left\{1-\frac{D}{D_0}\right\}+\frac{D}{D_0}\nu_{f23}\right)\right\}
\end{aligned}
\tag{38}
$$

where E_{33C} is given by equation (26).
By adding the above three contributions the total microstress in region B is obtained as

$$
\sigma_{m33C} = \sigma^{(1)}_{m33C} + \sigma^{(2)}_{m33C} + \sigma^{(3)}_{m33C} \tag{39}
$$

The Region A stresses are given by

$$
\begin{aligned}
\sigma_{m33A}^{(3)} &= \sigma_{l33}\frac{E_{m33A}}{E_{l33}} \\
\sigma_{m33A}^{(1)} &= -\sqrt{k_f}\left[\left\{1-\frac{D}{D_0}\right\}\sigma_{m33B}^{(1)} + \frac{D}{D_0}\sigma_{m33C}^{(1)}\right] \\
\sigma_{m33A}^{(2)} &= -\sqrt{k_f}\left[\left\{1-\frac{D}{D_0}\right\}\sigma_{m33B}^{(2)} + \frac{D}{D_0}\sigma_{m33C}^{(2)}\right] \\
\sigma_{m33A} &= \sigma_{m33A}^{(1)} + \sigma_{m33A}^{(2)} + \sigma_{m33A}^{(3)}
\end{aligned}
\tag{40}
$$

Interphase microstresses due to applied ply normal stresses

Stresses along the longitudinal (11) direction in Region B: The interphase longitudinal stresses due to the three normal applied ply stresses in the Region B are given by

$$
\begin{aligned}
\sigma_{d11B}^{(1)} &= E_{d11B}\frac{\sigma_{l11}}{E_{l11}} \\
\sigma_{d11B}^{(2)} &= -(\nu_{l21}-\nu_{d21B})\frac{E_{d11B}}{E_{l22}}\sigma_{l22} \\
\sigma_{d11B}^{(3)} &= -(\nu_{l31}-\nu_{d31B})\frac{E_{d11B}}{E_{l33}}\sigma_{l33} \\
\sigma_{d11B} &= \sigma_{d11B}^{(1)} + \sigma_{d11B}^{(2)} + \sigma_{d11B}^{(3)}
\end{aligned}
\tag{41}
$$

Stresses along the longitudinal (11) direction in Region C: These are obtained by changing the subscript B to C in the above equations. Accordingly, these are given by

$$
\begin{aligned}
\sigma_{d11C}^{(1)} &= E_{d11C}\frac{\sigma_{l11}}{E_{l11}} \\
\sigma_{d11C}^{(2)} &= -(\nu_{l21}-\nu_{d21C})\frac{E_{d11C}}{E_{l22}}\sigma_{l22} \\
\sigma_{d11C}^{(3)} &= -(\nu_{l31}-\nu_{d31C})\frac{E_{d11C}}{E_{l33}}\sigma_{l33} \\
\sigma_{d11C} &= \sigma_{d11C}^{(1)} + \sigma_{d11C}^{(2)} + \sigma_{d11C}^{(3)}
\end{aligned}
\tag{42}
$$

Stresses along the transverse (22 and 33) direction in Regions B and C: These are same as the matrix microstresses in the regions B and C.

$$
\begin{aligned}
\sigma_{d22B} &= \sigma_{m22B} \\
\sigma_{d22C} &= \sigma_{m22C} \\
\sigma_{d33B} &= \sigma_{m33B} \\
\sigma_{d33C} &= \sigma_{m33C}
\end{aligned}
\tag{43}
$$

The above completes the discussion on constituent microstresses in various Regions A, B, and C. It should be noted that the mircrostresses due to temperature differential must be added to those due to mechanical loads to obtain the combined microstresses due to thermo-mechanical loading.

Apart from these microstresses which are basically the stresses due to normal loads, there exist the shear stresses due to the applied shear force resultants. These are also obtained in a similar fashion and are given in the following paragraphs.

Fiber microstresses due to applied ply shear stresses

The fiber microstresses due to the three applied ply shear stresses are given by

$$
\begin{aligned}
\sigma_{f12} &= \frac{\sigma_{l12}\dfrac{G_{f12}}{G_{l12}}}{\left(1.-\sqrt{k_f}\left\{1-(1-\dfrac{D}{D_0})\dfrac{G_{m12}}{G_{d12}}-(\dfrac{D}{D_0})\dfrac{G_{m12}}{G_{f12}}\right\}\right)} \\
\sigma_{f13} &= \frac{\sigma_{l13}\dfrac{G_{f13}}{G_{l13}}}{\left(1.-\sqrt{k_f}\left\{1-(1-\dfrac{D}{D_0})\dfrac{G_{m13}}{G_{d13}}-(\dfrac{D}{D_0})\dfrac{G_{m13}}{G_{f13}}\right\}\right)} \\
\sigma_{f23} &= \frac{\sigma_{l23}\dfrac{G_{f23}}{G_{l23}}}{\left(1.-\sqrt{k_f}\left\{1-(1-\dfrac{D}{D_0})\dfrac{G_{m23}}{G_{d23}}-(\dfrac{D}{D_0})\dfrac{G_{m23}}{G_{f23}}\right\}\right)}
\end{aligned}
\tag{44}
$$

Matrix microstresses due to applied ply shear stresses

Region A: The matrix microstresses due to the three applied ply shear stresses are given by

$$
\sigma_{m12A} = \sigma_{l12}\frac{G_{m12A}}{G_{l12}} \; ; \; \sigma_{m13A} = \sigma_{l13}\frac{G_{m13A}}{G_{l13}} \; ; \; \sigma_{m23A} = \sigma_{l23}\frac{G_{m23A}}{G_{l23}}
\tag{45}
$$

Region B: The microstresses in region B due to the three applied ply shear stresses are calculated by

$$\sigma_{m12B} = \sigma_{l12}\frac{\dfrac{G_{m12B}}{G_{l12}}}{1-\sqrt{k_f}\left(1-\dfrac{G_{m12}}{G_{d12}}\right)}$$

$$\sigma_{m13B} = \sigma_{l13}\frac{\dfrac{G_{m13B}}{G_{l13}}}{1-\sqrt{k_f}\left(1-\dfrac{G_{m13}}{G_{d13}}\right)} \tag{46}$$

$$\sigma_{m23B} = \sigma_{l23}\frac{\dfrac{G_{m23B}}{G_{l23}}}{1-\sqrt{k_f}\left(1-\dfrac{G_{m23}}{G_{d23}}\right)}$$

Region C: The region C stresses are calculated by

$$\sigma_{m12C} = \sigma_{l12}\frac{\dfrac{G_{m12C}}{G_{l12}}}{\left[1-\sqrt{k_f}\left(1-(1-\dfrac{D}{D_0})\dfrac{G_{m12}}{G_{d12}}-\dfrac{D}{D_0}\dfrac{G_{m12}}{G_{f12}}\right)\right]}$$

$$\sigma_{m13C} = \sigma_{l13}\frac{\dfrac{G_{m13C}}{G_{l13}}}{\left[1-\sqrt{k_f}\left(1-(1-\dfrac{D}{D_0})\dfrac{G_{m13}}{G_{d13}}-\dfrac{D}{D_0}\dfrac{G_{m13}}{G_{f13}}\right)\right]} \tag{47}$$

$$\sigma_{m23C} = \sigma_{l23}\frac{\dfrac{G_{m23C}}{G_{l23}}}{\left[1-\sqrt{k_f}\left(1-(1-\dfrac{D}{D_0})\dfrac{G_{m23}}{G_{d23}}-\dfrac{D}{D_0}\dfrac{G_{m23}}{G_{f23}}\right)\right]}$$

<u>Interphase microstresses due to applied ply shear stresses</u>

Region B: The region B interphase stresses are calculated from

$$\sigma_{d12B} = \sigma_{l12} \frac{\dfrac{G_{d12B}}{G_{l12}}}{1-\sqrt{k_f}\left(1-\dfrac{G_{m12}}{G_{d12}}\right)}$$

$$\sigma_{d13B} = \sigma_{l13} \frac{\dfrac{G_{d13B}}{G_{l13}}}{1-\sqrt{k_f}\left(1-\dfrac{G_{m13}}{G_{d13}}\right)} \tag{48}$$

$$\sigma_{d23B} = \sigma_{l23} \frac{\dfrac{G_{d23B}}{G_{l23}}}{1-\sqrt{k_f}\left(1-\dfrac{G_{m23}}{G_{d23}}\right)}$$

Region C: The region C stresses are given by

$$\sigma_{d12C} = \sigma_{l12} \frac{\dfrac{G_{d12C}}{G_{l12}}}{\left[1-\sqrt{k_f}\left(1-(1-\dfrac{D}{D_0})\dfrac{G_{m12}}{G_{d12}}-\dfrac{D}{D_0}\dfrac{G_{m12}}{G_{f12}}\right)\right]}$$

$$\sigma_{d13C} = \sigma_{l13} \frac{\dfrac{G_{d13C}}{G_{l13}}}{\left[1-\sqrt{k_f}\left(1-(1-\dfrac{D}{D_0})\dfrac{G_{m13}}{G_{d13}}-\dfrac{D}{D_0}\dfrac{G_{m13}}{G_{f13}}\right)\right]} \tag{49}$$

$$\sigma_{d23C} = \sigma_{l23} \frac{\dfrac{G_{d23C}}{G_{l23}}}{\left[1-\sqrt{k_f}\left(1-(1-\dfrac{D}{D_0})\dfrac{G_{m23}}{G_{d23}}-\dfrac{D}{D_0}\dfrac{G_{m23}}{G_{f23}}\right)\right]}$$

This completes the equations for microstresses due to applied ply shear stresses. Overall, there are six fiber microstresses (three normal and three shear), 18 matrix microstresses (nine normal and nine shear), and 12 interphase microstresses (six normal and six shear) that result due to the six ply stresses (three normal and three shear). The ply stresses are calculated in the subroutine COMSA using classical lamination theory for each incremental load step. These are then passed to the microstress module comprised of the subroutines STRESI, STRESF, STRESM and STRESD for the computation of the incremental microstresses which are cumulatively added to obtain the total microstress in each constituent and in each region. These microstresses are input to the MFIR module for calculating the stress dependence of the constituent material behavior. Also, at the end of each computation, these microstresses are compared with the respective allowable strengths (e. g. σ_{f11} is compared with $S_{f11T,C}$) to check for any failures in the constituents. If a particular constituent shows stress failure, its respective stiffness is equated to a negligible value (e.g. E_{f11} = 0.01 psi) in order redistribute the load and change its path.

Micromechanics

Composite micromechanics theory refers to the collection of physical principles, mathematical models, assumptions and approximations employed to relate the behavior of a simple composite unit (e.g., lamina or ply) to the behavior of its individual constituents. The primary objective of composite micromechanics is to determine the equivalent mechanical, and thermal properties of a composite ply in terms of the properties of the constituent materials. The mechanical properties refer to normal moduli, shear moduli, and Poisson's ratios. The thermal properties include the thermal conductivities, heat capacity and the coefficients of thermal expansion. The derivation of equivalent composite ply properties using micromechanics theory starts with the identification of a representative volume element or unit cell as shown in Figure 5. It is the smallest region or piece of material over which the stresses and strains are macroscopically uniform. However, within the unit cell the stresses and strains are nonuniform due to the heterogeneity of the material. The unit cell can consist of a fiber, matrix and/or an interphase. It is assumed that these cells are arranged in a regular square array pattern. Equivalent properties for the ply are then derived in terms of the constituent material properties based on the mechanics of materials approach. Other assumptions involved in this approach are: 1) fiber and matrix are subjected to the same strain in the fiber direction of a unidirectional fibrous composite, and 2) the same transverse stress is applied to both the fiber and matrix in the direction transverse to the fiber.

Physical Properties

The mass density of the ply is assumed to be given by the rule of mixtures type equation as shown below:

$$\rho_l = k_f\rho_f + k_m\rho_m + (1-k_f-k_m)\rho_d \tag{50}$$

The above is calclulated in the subroutine PLYMAT.

Mechanical Properties

The micromechanics equations which facilitate the computation of ply equivalent properties are programmed in the subroutine MECHPL in METCAN. The actual details of derivations for the ply longitudinal and transverse moduli are given in the Appendix. The derivation of the remaining properties follow along the same lines as described in the Appendix. The following is a brief list of the various equations:

Ply Normal Moduli: The longitudinal modulus E_{l11} of the ply is calculated based on the assumption that the compatibility of longitudinal displacement requires equal strains for the composite and constituents [1]:

$$E_{l11} = k_m E_{m11} + k_f \left[E_{d11}\left(1-\left\{\frac{D}{D_0}\right\}^2\right) + E_{f11}\left\{\frac{D}{D_0}\right\}^2 \right] \tag{50}$$

The transverse normal moduli E_{l22} and E_{l33} are derived by first computing the equivalent moduli in each of the regions A, B and C and then combining them by assuming that the subregions act as parallel elements when subjected to a transverse load. To compute the equivalent moduli of each subregion it is assumed that the stress due to transverse load is same in each of the constituents. This leads to the following expressions for the transverse moduli:

$$E_{l22} = E_{m22}\left[1-\sqrt{k_f}+\frac{\sqrt{k_f}\left(1-\frac{D}{D_0}\right)}{\left\{1-\sqrt{k_f}\left(1-\frac{E_{m22}}{E_{d22}}\right)\right\}} + \frac{\sqrt{k_f}\left(\frac{D}{D_0}\right)}{\left[1-\sqrt{k_f}\left(1-\left(1-\frac{D}{D_0}\right)\frac{E_{m22}}{E_{d22}}-\frac{D}{D_0}\frac{E_{m22}}{E_{f22}}\right)\right]}\right] \tag{51}$$

$$E_{l33} = E_{m33}\left[1-\sqrt{k_f}+\frac{\sqrt{k_f}\left(1-\frac{D}{D_0}\right)}{\left\{1-\sqrt{k_f}\left(1-\frac{E_{m33}}{E_{d33}}\right)\right\}} + \frac{\sqrt{k_f}\left(\frac{D}{D_0}\right)}{\left[1-\sqrt{k_f}\left(1-\left(1-\frac{D}{D_0}\right)\frac{E_{m33}}{E_{d33}}-\frac{D}{D_0}\frac{E_{m33}}{E_{f33}}\right)\right]}\right] \tag{52}$$

Ply Shear Moduli:
The derivation for the shear moduli in 1-2 and 1-3 directions follow along the same lines as that of the transverse modulus. The shear modulus in 1-2 direction is given by

$$G_{l12} = G_{m12}\left[1-\sqrt{k_f}+\frac{\sqrt{k_f}\left(1-\frac{D}{D_0}\right)}{\left\{1-\sqrt{k_f}\left(1-\frac{G_{m12}}{G_{d12}}\right)\right\}} + \frac{\sqrt{k_f}\left(\frac{D}{D_0}\right)}{\left[1-\sqrt{k_f}\left(1-\left(1-\frac{D}{D_0}\right)\frac{G_{m12}}{G_{d12}}-\frac{D}{D_0}\frac{G_{m12}}{G_{f12}}\right)\right]}\right] \tag{53}$$

The shear modulus in 1-3 direction is given by

$$G_{l13} = G_{m13}\left[1-\sqrt{k_f}+\frac{\sqrt{k_f}(1-\frac{D}{D_0})}{\left\{1-\sqrt{k_f}(1-\frac{G_{m13}}{G_{d13}})\right\}}+\frac{\sqrt{k_f}(\frac{D}{D_0})}{\left[1-\sqrt{k_f}\left(1-(1-\frac{D}{D_0})\frac{G_{m13}}{G_{d13}}-\frac{D}{D_0}\frac{G_{m13}}{G_{f13}}\right)\right]}\right] \tag{54}$$

The shear modulus in 2-3 direction is calculated by utilizing the transverse isotropy in the 2-3 direction:

$$G_{l23} = \frac{E_{l22}}{2(1 + \nu_{l23})} \tag{55}$$

Alternatively, shear modulus in the 2-3 direction can also be derived independently using the same criteria as that of transverse modulus derivation. It is given by

$$G_{l23} = \frac{G_{m23}}{\left[(1-\sqrt{k_f}) + \sqrt{k_f}\left(1-\frac{D}{D_0}\right)\right]\left\{1-\sqrt{k_f}\left(1-\frac{G_{m23}}{G_{d23}}\right)\right\} + \sqrt{k_f}\frac{D}{D_0}\left\{1-\sqrt{k_f}+\sqrt{k_f}\left[\left(1-\frac{D}{D_0}\right)\frac{G_{m23}}{G_{d23}}+\frac{D}{D_0}\frac{G_{m23}}{G_{f23}}\right]\right\}} \tag{56}$$

Note that currently in METCAN this equation is not used.

Poisson's Ratios: The derivation for the major Poisson's ratio in 1-2 and 1-3 direction follow the derivation for the longitudinal modulus where in the fiber and matrix elements are assumed to be acting in parallel. The respective equations are

$$\nu_{l12} = k_m\nu_{m12} + k_f\left[\left(1-\left\{\frac{D}{D_0}\right\}^2\right)\nu_{d12} + \left\{\frac{D}{D_0}\right\}^2\nu_{f12}\right] \tag{57}$$

$$\nu_{l13} = k_m\nu_{m13} + k_f\left[\left(1-\left\{\frac{D}{D_0}\right\}^2\right)\nu_{d13} + \left\{\frac{D}{D_0}\right\}^2\nu_{f13}\right] \tag{58}$$

Poisson's Ratio in 2-3 direction: The Poisson's ratio in 2-3 direction is derived by using a combination of series and parallel elements of the various subregions A, B and C. The equation is given by

$$\nu_{l23}=(1-\sqrt{k_f})\nu_{m23}^{A}+\frac{\sqrt{k_f}\left(1-\frac{D}{D_0}\right)E_{m22}^{B}}{\left[1-\sqrt{k_f}\left(1-\frac{E_{m22}^{B}}{E_{d22}^{B}}\right)\right]}\left[\frac{(1-\sqrt{k_f})\nu_{m23}^{B}}{E_{m22}^{B}}+\frac{\sqrt{k_f}\,\nu_{d22}^{B}}{E_{d22}^{B}}\right]$$

$$+\frac{\sqrt{k_f}\,E_{m22}^{C}\frac{D}{D_0}}{1-\sqrt{k_f}\left[1-\left(1-\frac{D}{D_0}\right)\frac{E_{m22}^{C}}{E_{d22}^{C}}-\frac{D}{D_0}\frac{E_{m22}^{C}}{E_{f22}}\right]}\left[\frac{(1-\sqrt{k_f})\nu_{m23}^{C}}{E_{m22}^{C}}+\frac{\sqrt{k_f}\left(1-\frac{D}{D_0}\right)\nu_{d23}^{C}}{E_{d22}^{C}}+\frac{\sqrt{k_f}\frac{D}{D_0}\nu_{f23}}{E_{f22}}\right] \tag{59}$$

Thermal Properties:

The properties under this category are the three thermal expansion coefficients, the three thermal conductivities and the heat capacity. These are computed in the subroutine THERMPL in METCAN.

Longitudinal thermal expansion coefficient: This is derived based on the observation that free expansion in 1-1 direction produces no resultant load in that direction. This implies that the integrated effect over the cross section of the sum of the individual stresses developed in each constituent due to the mismatch of the thermal expansion coefficients must add up to zero identically. This leads to the following expression for the longitudinal thermal expansion coefficient:

$$\alpha_{l11} = k_m\frac{E_m}{E_{l11}}\alpha_{m11} + k_f\left\{1-\left(\frac{D}{D_0}\right)^2\right\}\frac{E_d}{E_{l11}}\alpha_{d11} + \left(\frac{D}{D_0}\right)^2 k_f\frac{E_f}{E_{l11}}\alpha_{f11} \tag{60}$$

Transverse thermal expansion coefficients: The derivation for the transverse thermal expansion coefficients is carried in two stages analogous to the derivation of the transverse moduli. First, equivalent thermal expansion coefficients are written for each subregion A, B, and C. During this stage the individual constituents are assumed to act in series. The overall equivalent thermal expansion for the unit cell is then written by assuming the individual regions to act in parallel. The following are the equations for the two transverse thermal expansion coefficients:

$$\alpha_{l22} = \frac{E_m}{E_{l22}} \left[(1-\sqrt{k_f})\alpha_{m22} + \frac{\left\{1-\frac{D}{D_0}\right\}\left\{(1-\sqrt{k_f})\alpha_{m22} + \sqrt{k_f}\alpha_{d22}\right\}}{1-\sqrt{k_f}\left(1-\frac{E_{m22}}{E_{d22}}\right)} \right.$$

$$\left. + \frac{\sqrt{k_f}\alpha_{m22} - k_f\left\{\alpha_{m22} - \left(1-\frac{D}{D_0}\right)\alpha_{d22} - \frac{D}{D_0}\alpha_{f22}\right\}}{1-\sqrt{k_f}\left\{1-\left(1-\frac{D}{D_0}\right)\frac{E_{m22}}{E_{d22}} - \frac{D}{D_0}\frac{E_{m22}}{E_{f22}}\right\}} \right] \tag{61}$$

$$\alpha_{l33} = \frac{E_m}{E_{l33}} \left[(1-\sqrt{k_f})\alpha_{m33} + \frac{\left\{1-\frac{D}{D_0}\right\}\left\{(1-\sqrt{k_f})\alpha_{m33} + \sqrt{k_f}\alpha_{d33}\right\}}{1-\sqrt{k_f}\left(1-\frac{E_{m33}}{E_{d33}}\right)} \right.$$

$$\left. + \frac{\sqrt{k_f}\alpha_{m33} - k_f\left\{\alpha_{m33} - \left(1-\frac{D}{D_0}\right)\alpha_{d33} - \frac{D}{D_0}\alpha_{f33}\right\}}{1-\sqrt{k_f}\left\{1-\left(1-\frac{D}{D_0}\right)\frac{E_{m33}}{E_{d33}} - \frac{D}{D_0}\frac{E_{m33}}{E_{f33}}\right\}} \right] \tag{62}$$

Longitudinal heat conductivity: The longitudinal heat conductivity of the ply is derived by assuming that the three constituents are in parallel which yields the following rule of mixtures type expression:

$$K_{l11} = k_m K_{m11} + k_f\left\{\left[1-\left(\frac{D}{D_0}^2\right)\right]K_{d11} + \left(\frac{D}{D_0}\right)^2 K_{f11}\right\} \tag{63}$$

Transverse heat conductivities: To derive the transverse conductivities the approach adopted for the derivation of the transverse moduli is followed. The equivalent heat conductivity for each subregion A, B and C is first expressed assuming that the constituents are acting in series followed by the expression of the ply conductivity assuming that each subregion is acting in parallel. This yields the following expressions for the transverse conductivities:

$$K_{l22} = K_{m22}\left[1-\sqrt{k_f}+\frac{\sqrt{k_f}(1-\frac{D}{D_0})}{\left\{1-\sqrt{k_f}(1-\frac{K_{m22}}{K_{d22}})\right\}}+\frac{\sqrt{k_f}(\frac{D}{D_0})}{\left[1-\sqrt{k_f}\left(1-(1-\frac{D}{D_0})\frac{K_{m22}}{K_{d22}}-\frac{D}{D_0}\frac{K_{m22}}{K_{f22}}\right)\right]}\right] \quad (64)$$

$$K_{l33} = K_{m33}\left[1-\sqrt{k_f}+\frac{\sqrt{k_f}(1-\frac{D}{D_0})}{\left\{1-\sqrt{k_f}(1-\frac{K_{m33}}{K_{d33}})\right\}}+\frac{\sqrt{k_f}(\frac{D}{D_0})}{\left[1-\sqrt{k_f}\left(1-(1-\frac{D}{D_0})\frac{K_{m33}}{K_{d33}}-\frac{D}{D_0}\frac{K_{m33}}{K_{f33}}\right)\right]}\right] \quad (65)$$

Heat capacity: The equivalent ply heat capacity is obtained by the simple rule of mixtures type equation.

$$C_l = k_m\frac{\rho_m}{\rho_l}C_m + k_f\left\{1-\left(\frac{D}{D_0}\right)^2\right\}\frac{\rho_d}{\rho_l}C_d + \left(\frac{D}{D_0}\right)^2\frac{\rho_f}{\rho_l}C_f \quad (66)$$

where ρ_l is the equivalent ply density.

Macromechanics

Macromechanics is the study of composite behavior wherein the material is presumed homogeneous and the effects of the constituent materials are detected only as averaged apparent properties of the composite. Thus, a collection of procedures which allows to proceed from the lamina or ply level properties to the global or laminate level properties where the heterogeneities associated with fiber, matrix and interphase are completely smeared out constitutes the theory of macromechanics. These procedures utilize the classical laminate theory to integrate the ply level properties and obtain the laminate level properties. These procedures are well known and are explained thoroughly in many text books. Therefore they are not repeated here. References [4-5] may be consulted for the theoretical details. Also, Reference [6] may be consulted for how these procedures are incorporated in METCAN, as many of these subroutines are taken from the earlier computer code ICAN which was primarily developed for polymer matrix composites. The principal subroutines that perform the macromechanical integration in METCAN are GACD3, GPCFD2 and COMSA. These are essentially the same subroutines that are used in ICAN [6,7].

Incremental Iterative Solution Scheme

The nonlinear thermo-mechanical response of high temperature metal matrix composites is obtained using an incremental iterative solution scheme as shown in the flow chart in Figure 6. During each load increment a linear laminate analysis is performed. At the end of each such analysis the response is saved and compared with that of the previous step till convergence to a prescribed tolerance level is achieved. The properties of the constituents are varied in each iteration based upon the current response and temperature using the multi-factor-interaction-relationship. A different flow chart is shown in figure 7 which indicates the principal subroutines of the program that are active in each of the blocks shown in figure 6. Note that in this flow chart the modules performing output operations are intentionally removed to avoid clutter. Only the basic operations pertaining to nonlinear material model, micromechanics and macromechanics are indicated. This chart should be consulted along with figure 2 by those wishing to debug/update/modify the code.

Convergence Criteria

The convergence criteria used in METCAN is based on the global/laminate level strains. During each incremental load step analysis, the global incremental strains are preserved and are compared between successive iterations. If the differences are with in five percent convergence is assumed to have been achieved. The tolerance level is hard wired in the code. However, it can be easily altered. Also, alternative convergence criteria based on ply level strains/stresses/properties can be set with out much difficulty.

Concluding Remarks

The computer code METCAN is developed for simulating the nonlinear behavior of high temperature metal matrix composites. The code documentation consists of a set of three manuals. They deal with the code usage, demonstration of the code capabilities and the theoretical aspects pertaining to the high temperature metal matrix micromechanics. The present manual provides a summary of all the theoretical details embedded in the computer code METCAN. The emphasis, however, is placed specifically on the micromechanics, microstresses and the nonlinear material behavior models that are incorporated in METCAN. The primary intention is to provide information to the code user who might want to modify, update, and debug the code. Assumptions leading to the derivation of various equations are briefly mentioned with no details on the actual procedure. The details of the derivation is beyond the scope of the present manual. The actual usage of the computer code is discussed in the companion volume "METCAN User's Manual. The various features of the code and how they can be utilized are discussed in the companion volume "METCAN Demonstration Manual". For a complete understanding of the code and its capabilities the user is advised to refer to all the three volumes.

Appendix

In order to demonstrate the formal procedure involved in the application of composite micromechanics theory, derivations of the equations for ply normal moduli (E_{l11} and E_{l22}) are explicitly developed below. The particular approach taken here relies on the principles of force equilibrium and displacement compatibility as defined from elementary mechanics of materials approach.

<u>Longitudinal Modulus</u>
Consider a square array unit cell model (see Fig. 5) subjected to a uniaxial load in the longitudinal direction. The equivalent composite (ply) load is defined from force equilibrium to be the sum of the constituent loads as follows:

$$P_f = P_f + P_d + P_m \tag{1}$$

In the integrated average sense, Eq. (1) is rewritten as

$$\sigma_l A_l = \sigma_f A_f + \sigma_d A_d + \sigma_m A_m \tag{2}$$

where A represents cross sectional area. Division of the above equation by A_l followed by the substitution of the respective ratios of the areas with the volume fractions of the constituents the following can be written:

$$\sigma_l = \sigma_f k_f' + \sigma_d k_d + \sigma_m k_m \tag{3}$$

where k_f' is the actual fiber volume fraction based on the current fiber diameter D.
Since the compatibility of longitudinal displacement requires equal strains for the composite and constituents ($\epsilon_l = \epsilon_f = \epsilon_d = \epsilon_m$), Eq. (3) can be differentiated with respect to strain to give

$$\left(\frac{d\sigma_l}{d\epsilon}\right) = \left(\frac{d\sigma_f}{d\epsilon}\right)k_f' + \left(\frac{d\sigma_d}{d\epsilon}\right)k_d + \left(\frac{d\sigma_m}{d\epsilon}\right)k_m \tag{4}$$

The quantities ($d\sigma/d\epsilon$) represent the slopes of the corresponding stress strain curves for the composite and constituents and in this context define instantaneous of "tangent" moduli. Hence, Eq. (4) becomes

$$E_{l11} = E_f k_f' + E_d k_d + E_m k_m \tag{5}$$

The volume fractions can be expressed in terms of the inner and outer diameters of the fiber D and D_o and the apparent fiber volume ratio k_f.. Note that the apparent fiber volume ration is based on the original/outer diameter of the fiber D_o .

$$k_f' = k_f \left(\frac{D}{D_o}\right)^2$$

$$k_d = k_f \left\{1 - \left(\frac{D}{D_o}\right)^2\right\} \tag{6}$$

With the aid of equations (5) and (6) the following expression can be developed for the ply longitudinal modulus:

$$E_{l11} = E_f k_f \left(\frac{D}{D_0}\right)^2 + E_d k_f \left\{1 - \left(\frac{D}{D_o}\right)^2\right\} + E_m k_m \tag{7}$$

Transverse Normal Modulus in 2-2 direction

Consider the square array unit cell model again except that the fiber and interphase are of equivalent square cross section such that linear dimensions can be defined as follows:

$$a_f = \sqrt{\frac{\pi}{4}}\, D \; ; \; a_d = \sqrt{\frac{\pi}{4}}\, D_0 \; ; \; a_l = \sqrt{\frac{\pi}{4k_f}}\, D_0 \tag{8}$$

and

$$s_f = a_f \; ; \; s_d = a_d - a_f \; ; \; s_l = a_l \tag{9}$$

Assume a uniaxial load in the transverse direction and neglect Poisson"s effects. For the subregion C displacement compatibility yields

$$s_l \epsilon_l = s_f \epsilon_f + s_d \epsilon_d + s_m \epsilon_m \tag{10}$$

and the force equilibrium results in equal stresses for the composite and constituents ($\sigma_l = \sigma_f = \sigma_d = \sigma_m$). Hence, Eq. (10) can be differentiated with respect to stress to give

$$\left(\frac{d\epsilon_l}{d\sigma}\right) s_l = \left(\frac{d\epsilon_f}{d\sigma}\right) s_f + \left(\frac{d\epsilon_d}{d\sigma}\right) s_d + \left(\frac{d\epsilon_m}{d\sigma}\right) s_m \tag{11}$$

The quantities ($d\epsilon/d\sigma$) represent reciprocals of the slopes of the corresponding stress-strain curves for the composite and constituents and in the same context as before define reciprocals of instantaneous or "tangent" moduli. The above equation can be rearranged to yield the following:

$$E_l^C = \frac{E_m}{\left[\left(\frac{s_m}{s_l}\right) + \left(\frac{s_d}{s_l}\right)\left(\frac{E_m}{E_d}\right) + \left(\frac{s_f}{s_l}\right)\left(\frac{E_m}{E_f}\right)\right]} \tag{12}$$

With the aid of equations (7), (8) and (12) the equivalent modulus for the subregion C can be shown to be given by

$$E_l^C = \frac{E_m}{\left[1 - \sqrt{k_f}\left\{\left(1 - \frac{D}{D_o}\right) - \left(\frac{D}{D_o}\right)\left(\frac{E_m}{E_f}\right)\right\}\right]}$$

The equivalent modulus for subregion B can be deduced from Eq. (13) by letting D/D_o equal to unity. The result is

$$E_l^B = \frac{E_m}{\left[1 - \sqrt{k_f}\left\{1 - \left(\frac{E_m}{E_f}\right)\right\}\right]} \tag{14}$$

The equivalent modulus for subregion A is simply the matrix modulus or

$$E_l^A = E_m \tag{15}$$

The ply transverse modulus E_{l22} is defined by assuming that subregions A, B, and C act as parallel elements when subjected to a transverse load. This is analogous to the case for E_{l11} where the constituents are assumed to act in parallel. Hence, from Eq. 5 it can be deduced that

$$E_l s_l = E_l^C s_f + E_l^B s_d + E_l^A s_m \tag{16}$$

Division of the Eq. 16 by s_l, followed by the substitution of the equations (7) and (8) and the results from equations (13 - 16) leads to the following final expression for the transverse ply modulus E_{l22}.

$$E_{l22} = E_{m22}\left[1 - \sqrt{k_f} + \frac{\sqrt{k_f}\left(1 - \frac{D}{D_0}\right)}{\left\{1 - \sqrt{k_f}\left(1 - \frac{E_{m22}}{E_{d22}}\right)\right\}} + \frac{\sqrt{k_f}\left(\frac{D}{D_0}\right)}{\left[1 - \sqrt{k_f}\left(1 - \left(1 - \frac{D}{D_0}\right)\frac{E_{m22}}{E_{d22}} - \frac{D}{D_0}\frac{E_{m22}}{E_{f22}}\right)\right]}\right] \tag{17}$$

Note that in the above the subscripts f, m and d are replaced by "f22", "m22" and "d22" to indicate the direction of the loading.

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Table 1. METCAN units for constituent, ply and laminate properties

Property	Symbol	Unit
ELASTIC MODULUS	E	psi
SHEAR MODULUS	G	psi
POISSONS RATIO	ν	non-dim
THERM. EXP. COEFF.	α	in/in/F
DENSITY	ρ	lb/in**3
FIBER DIAMETER	D	in
HEAT CAPACITY	C	BTU/lb/F
HEAT CONDUCTIVITY	K	BTU-in/HR/in**2/F
STRENGTH	S	psi
THICKNESS	T	in
DISTANCE TO MIDPLANE	Z	in
ANGLE TO AXES	TH	degrees
TEMPERATURE	T	F
STRAIN	ϵ	in/in
STRESS	σ	psi
MEMBRANE LOADS	N	lb/in
BENDING LOADS	M	lb-in/in
FIBER VOLUME RATIO	k_f	non-dim

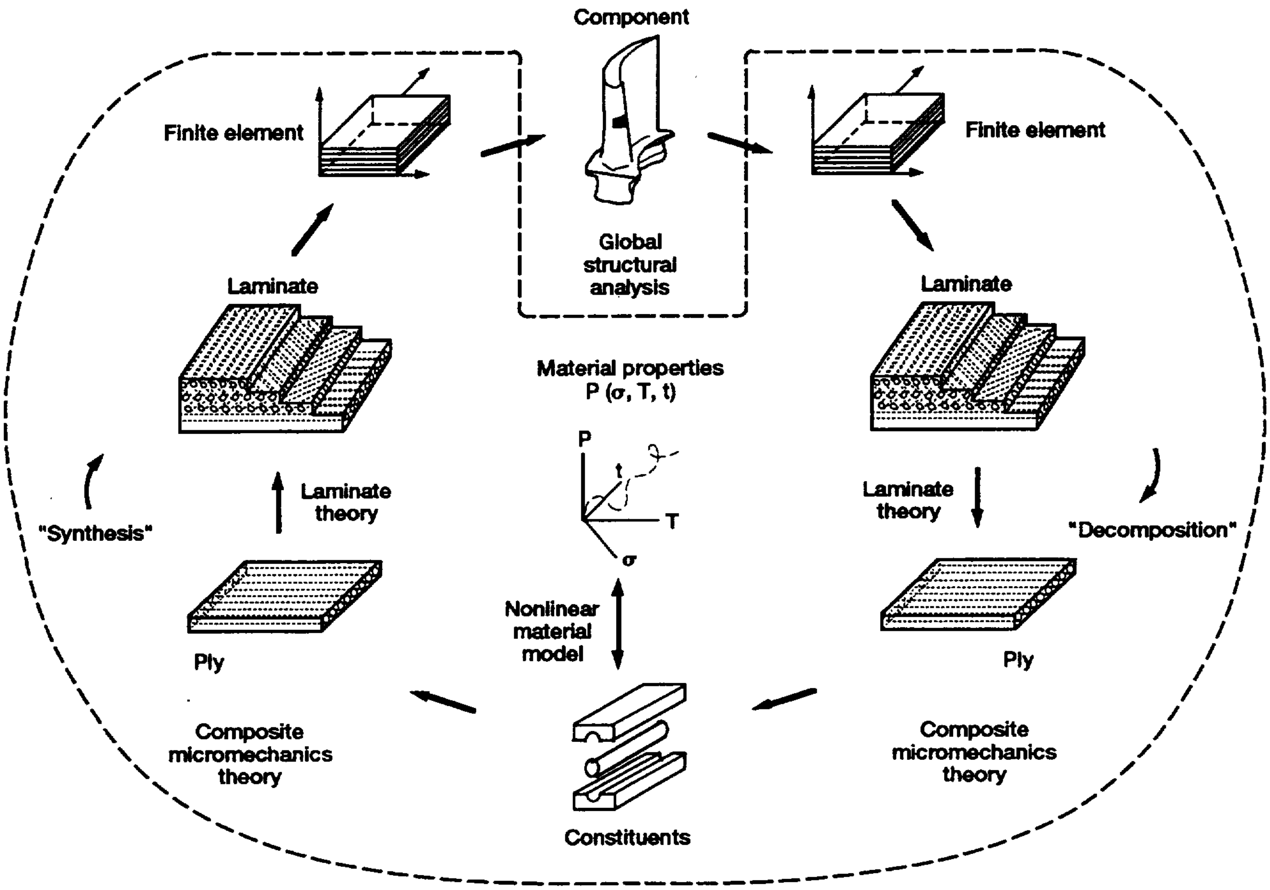
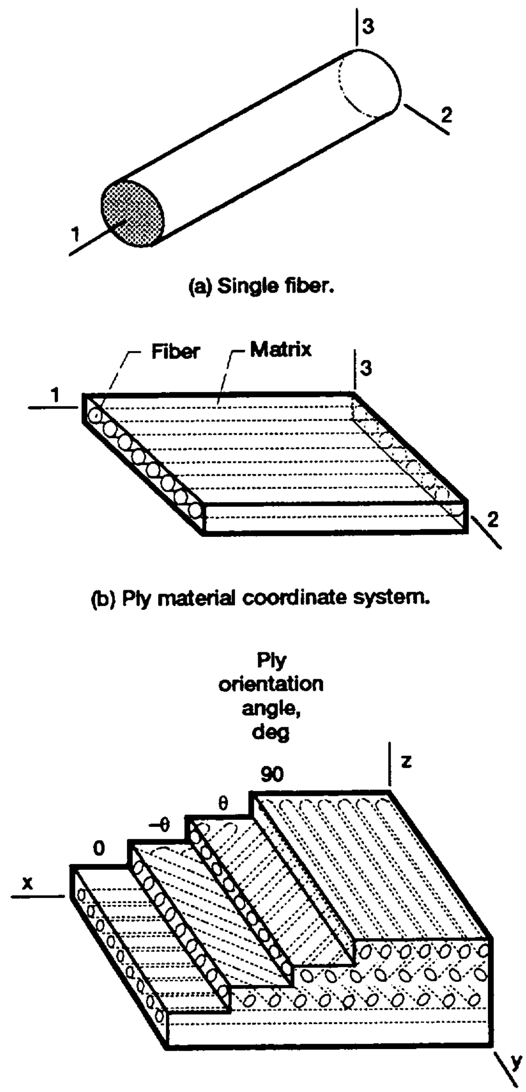


Figure 1.—Integrated multi-scale approach to metal matrix composite analysis.



(a) Single fiber.

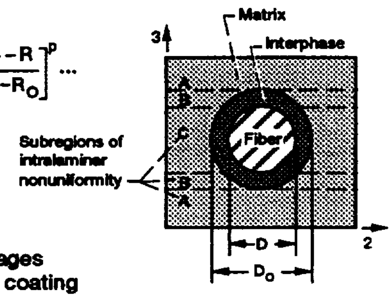
(b) Ply material coordinate system.

(c) Laminate structural coordinate system.

Figure 2.—Different coordinate systems used in METCAN.

$$\frac{P}{P_O} = \left[\frac{T_F - T}{T_F - T_O}\right]^n \left[\frac{S_F - \sigma}{S_F - \sigma_O}\right]^m \left[\frac{\dot{S}_F - \dot{\sigma}}{\dot{S}_F - \dot{\sigma}_O}\right]^\ell \left[\frac{\dot{T}_F - \dot{T}}{\dot{T}_F - \dot{T}_O}\right]^k \left[\frac{R_F - R}{R_F - R_O}\right]^p \ldots$$

$$\ldots \left[\frac{N_{MF} - N_M}{N_{MF} - N_{MO}}\right]^q \left[\frac{N_{TF} - N_R}{N_{TF} - N_{TO}}\right]^r \left[\frac{t_F - t}{t_F - t_O}\right]^s \ldots$$



Rationale:

- Gradual effects during most range, rapidly degrading near final stages
- Representative of the in situ behavior for fiber, matrix, interphase, coating
- Introduction of primitive variables (PV)
- Consistent in situ representation of all constituent properties in terms of PV
- Room–temperature values for reference properties
- Continuous interphase growth
- Simultaneous interaction of all primitive variables
- Adaptability to new materials
- Amenable to verification inclusive of all properties
- Readily adaptable to incremental computational simulation

Notations:

P – property; T – temperature; S – strength; R – metallurgical reaction; N – number of cycles:
t – time; over dot – rate; subscripts: O – reference; F – final; M – mechanical; T – thermal

Figure 3.—Assumed multifactor interaction relationship to represent the various factors which influence in situ constituent materials behavior.

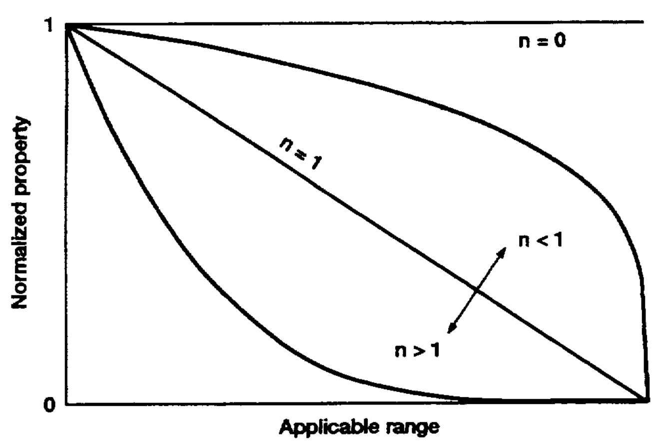


Figure 4.—Explanation of the multifactor interaction relationship.

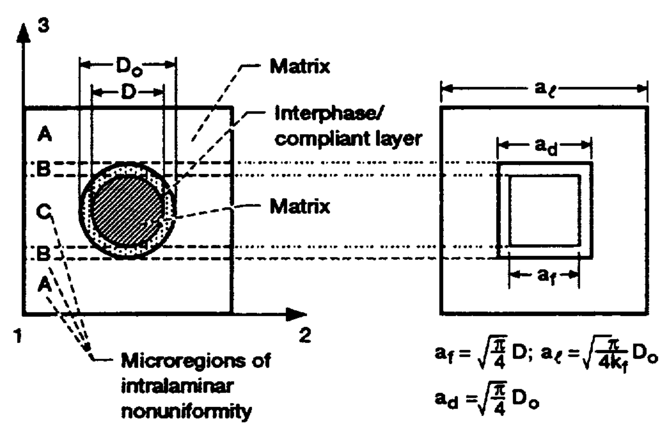


Figure 5.—METCAN unit cell showing the different regions A, B, and C of heterogenity and the idealization for the derivation of the micromechanical equations.

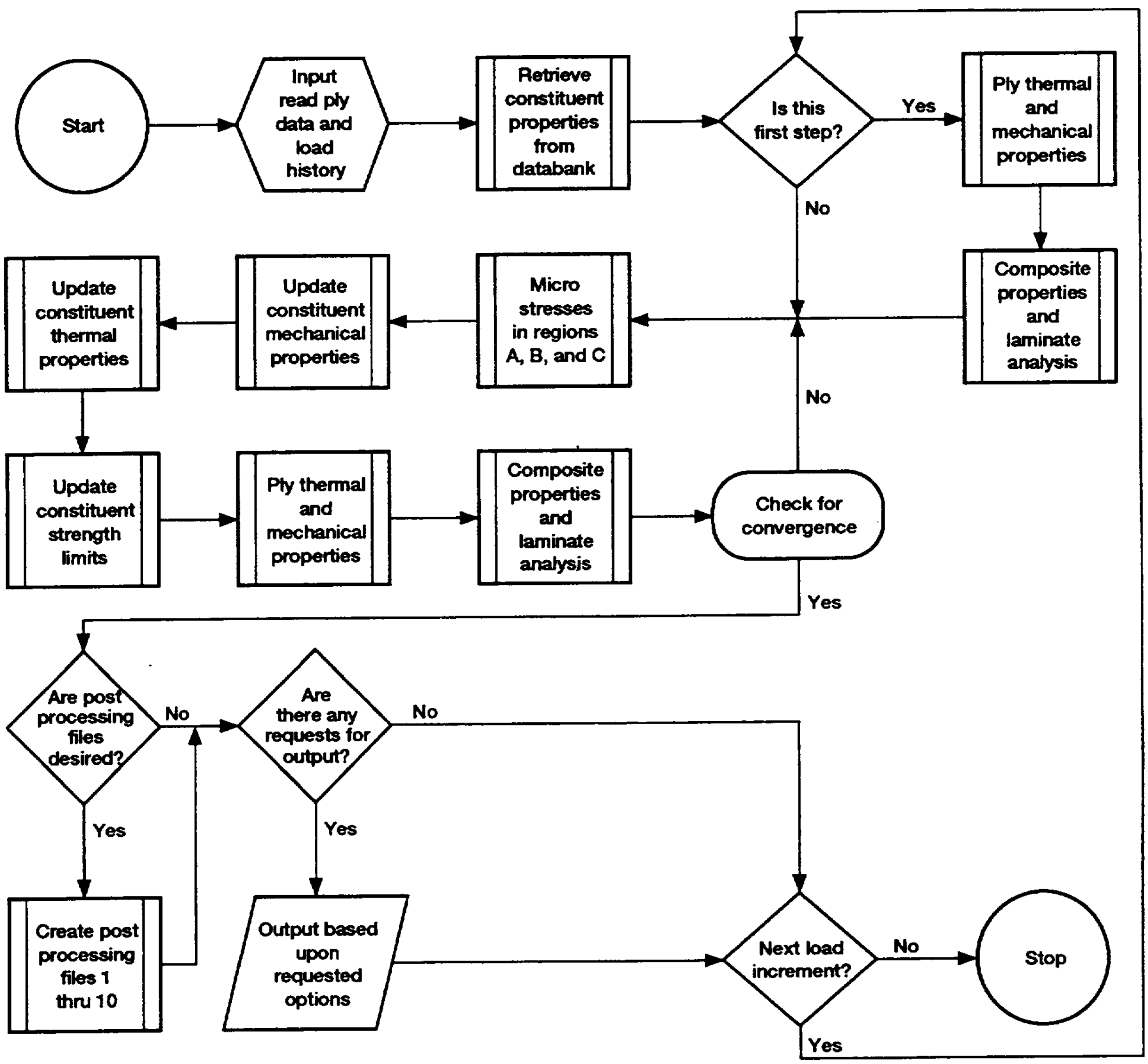


Figure 6.—METCAN flow chart.

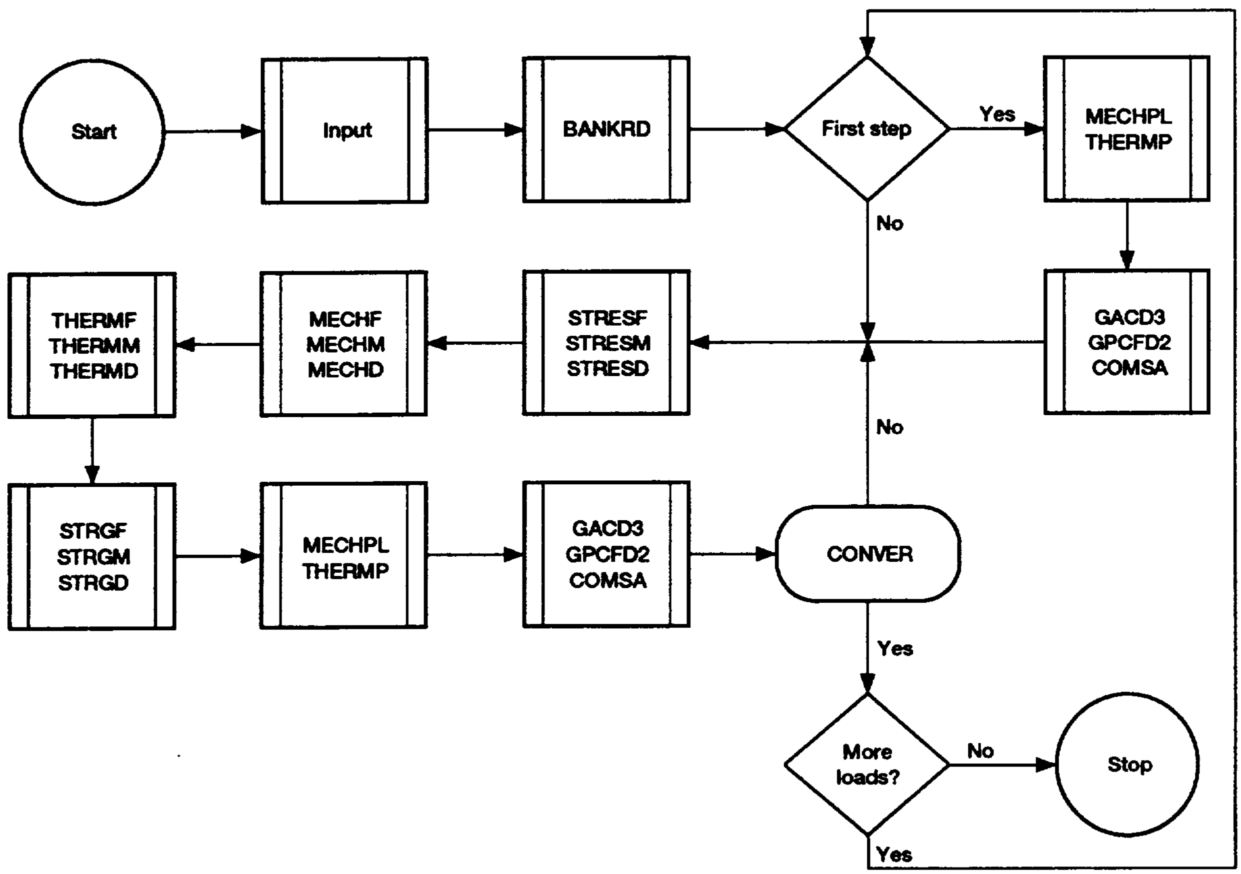


Figure 7.—METCAN flow chart showing the principal micromechanics and macromechanics routines.

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13. ABSTRACT ***(Maximum 200 words)***
This manuscript is intended to be a companion volume to the "METCAN User's Manual" and the "METCAN Demonstration Manual." The primary purpose of the manual is to give details pertaining to micromechanics and macromechanics equations of high temperature metal matrix composites that are programmed in the METCAN computer code. The subroutines which contain the programmed equations are also mentioned in order to facilitate any future changes or modifications that the user may intend to incorporate in the code. Assumptions and derivations leading to the micromechanics equations are briefly mentioned.

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