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In the first two-year effort, the effective modulus (homogenization) and size scales in composite laminate mechanics of severe stress gradients were examined in detail. We considered the issues regarding the homogenization of fiber-reinforced layers in a laminate in the presence of macroscopic (ply-level) stress gradients. A series of free edge boundary value problem were conducted. Despite the inability to provide such a homogenization theory, if one truly exists, we can devise approaches to predict the fiber/matrix interfacial stresses in an arbitrary cell by applying certain displacements and/or tractions on the cell boundaries. These boundary conditions were those derived by representing each layer in the laminate by conventional effective modulus theory (EMT). It has been shown that these primitive form of multi scale model can lead to reasonably accurate interfacial stresses and offer great promise as a means of solving practical laminate problems reinforced by fibers of moderate diameter.

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1. Abstract

The work in this project focused on multiscale modeling of composite laminates between the homogenized layer model and fiber/matrix micro-scale model in the region of high stress gradients. The goal was to develop a macroscopic theory, which can provide the connection between macromechanics (ply level) and micromechanics (fiber/matrix), especially in characterizing the micro-stress of composite laminates near edges and holes.

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With this confidence, a micropolar theory, a class of higher-order elasticity theory, of composite laminate mechanics was implemented. The micropolar homogenization method to determine the micropolar anisotropic effective elastic moduli was presented. A displacement-based finite element method based on micropolar theory in anisotropic solids was developed in analyzing composite laminates. The effects of fiber volume fraction and cell size on the normal stress along the artificial interface resulting from ply homogenization of the composite laminate were also investigated. The stress response based on micropolar theory was compared with those deduced from the micromechanics and classical elasticity theory. Special attention of the investigation focused on the stress fields near the free edge where the high macrostress gradient occurs. The normal stresses along the artificial interface and especially, the microstress along the fiber/matrix interface on the critical cell near the free edge where the high macrostress gradient detected were the focus of this investigation. These microstresses were expected to dominate the failure initiation process in composite laminate. A microstress recovery scheme based on micropolar analysis for the prediction of interface microstresses in the critical cell near the free edge was found to be in very good agreement with "exact" microstress solutions. It was demonstrated that the micropolar theory is able to capture the microstress accurately from the homogenized solutions.

From this multiscale modeling capable of zooming in the microstress from the macro (ply level) stresses near the high stress gradients, composite laminates can be potentially designed for aircraft and space applications with confidence, using only material properties as input. Micropolar theory can be used to establish realistic failure criteria for composite laminates in the presence of stress concentration by analysis and experiment at the micromechanical scale.

2. Technical Summary

Development and application of fiber reinforced composites have already witnessed phenomenal growth over the past two decades. The prospect of controlling a wide range of material microstructures and resulting properties has also been greatly enhanced. As the use of composite materials grows to include structural components, which are essential to the function and safety of engineering structures, a major need in the design of these composite laminates is to assess acceptable stress levels under the conditions to be experienced during service. Efficient use of the remarkable properties of fiber composites will expand even more rapidly if the material microstructure can further be precisely tailored to provide desired performance of composite structures.

Failure of composite laminates originated from micro-domain shown in the following figure. The analysis of failure in fiber composites has traditionally followed two different levels of abstraction. The areas of investigation are known as *micromechanics* and *macromechanics*.

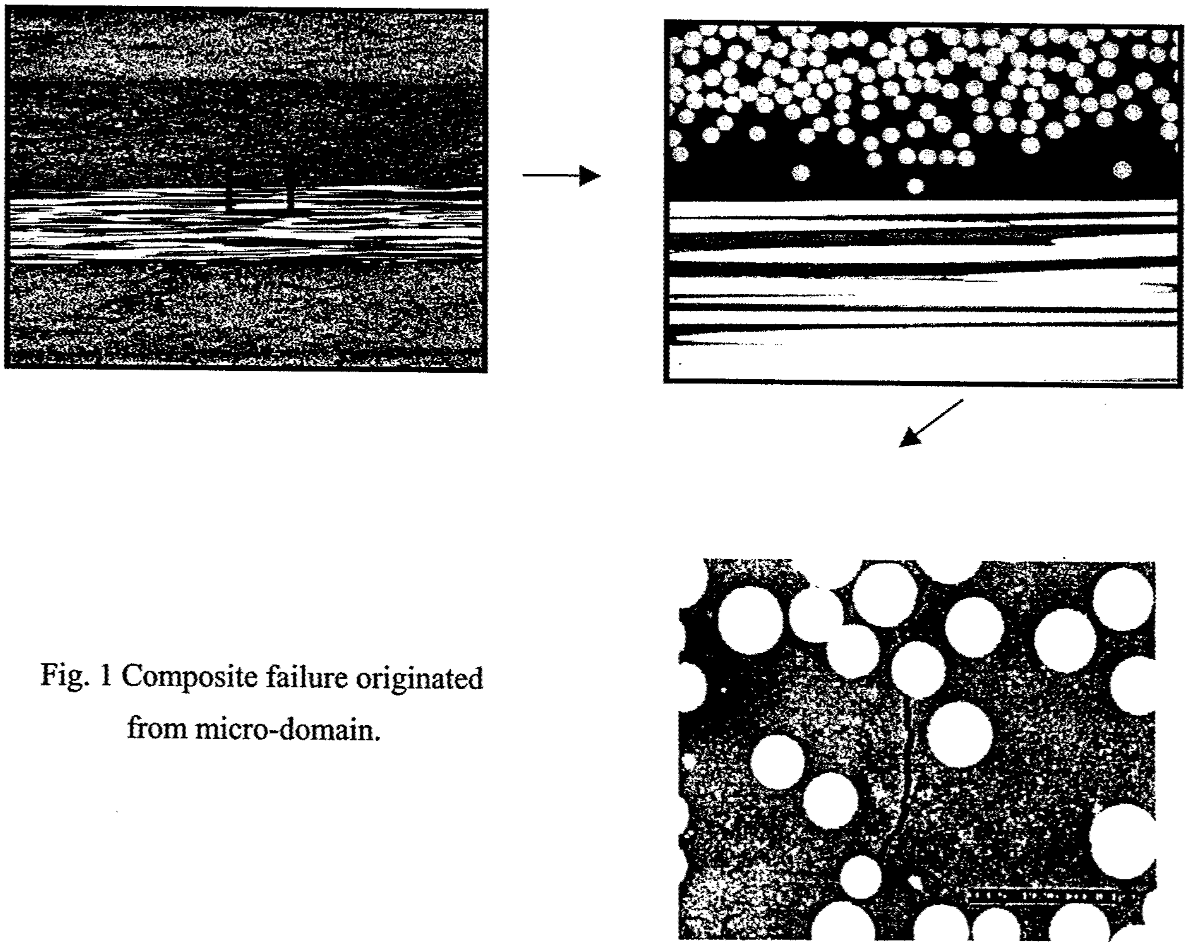


Fig. 1 Composite failure originated from micro-domain.

The micromechanics approach aims at the involvement of microscopic inhomogeneities in various kinds of micro-failure processes by taking the composite microstructure into account. The advantage of the micromechanics representation is that detailed information is directly obtained about the local interaction between the constituents and micro-failure mechanisms. The numerical modeling of exceedingly complicated geometric detail of all fibers and matrix, however, often requires exceedingly fine grids and hence results in excessive computer cost and capacity. The shear-lag model attempts to address this issue at a manageable level. However, this is done by oversimplifying the mechanical behavior of the constituents, which again leads to uncertain results. Even though many refinements have been incorporated into the shear-lag models, further progress requires an alternative approach. It is immediately obvious that conducting a stress analysis in realistic composite laminates with the presence of million of fibers using this approach is an almost impossible task beyond the computational capacity of even the latest supercomputers. Hence, the micromechanical model is mainly restricted to the strength prediction at the lamina level or unidirectional composites. The micromechanics analyses suffer from two main limitations. First, they are not able to provide quantitative predictions of failure in composites. Second, they cannot be applied to problems of engineering design importance such as failure in the presence of free edges or holes, mainly because the interlaminar stresses have been neglected in the failure processes.

From the existing analytical approaches, it is clear that micromechanics approach alone will not explain the failure process of the laminates simply because the mutual interaction between the micro-stresses and “interlaminar” macro-stresses in the failure process has been totally neglected. While in the macromechanics approach, although the macroscopic or overall constitutive descriptions are developed from composite microstructure in terms of the volume fraction, the shape, and the interface conditions of the constituents, the constitutive relations are independent of the scale of the microstructure. Further, the effective-modulus theory, in principle, only applies to macroscopically uniform fields. Therefore, the stress fields near the high stress gradient regions using the classical approximation are unreliable. Since the details of the generally complex, strongly heterogeneous microstructures are not considered directly, the conventional macroscopic theory would inevitably involve erroneous theoretical predictions, and from which precise information of failure in the micro-level would be difficult to elicit.

None of the currently available macroscopic theories can provide the connection between micromechanics and macromechanics in characterizing the elastic response of composite laminates near edges and holes. The ultimate failure of laminates, which intertwines with the micro-failure mechanisms, has to be quantified to provide the necessary theoretical basis for design and application of composites to structures. Furthermore, a systematic failure analysis requires a methodology at the macro-level to correctly determine the stress distributions near the high stress gradient locations at the micro-level. In addition, there is clearly a need for more comprehensive experimental studies of microstructural failure criteria, with emphasis on the requirements for applying predictive models to determine the ultimate load of the composite laminates.

Apparently, in regions of macroscopically steep stress (or strain) gradients such as free edges or holes, the conventional anisotropic elasticity theory utilizing the effective-modulus concept in the constitutive relations does not preserve the essential variation of the microstress distribution through the unit-cell at the micro-level. Indeed, rapid change of three-dimensional stress states contradicts the underlying assumption of the macroscopically uniform state of stress from which the effective-modulus theory has been derived. As a consequence, at regions of high stress gradient the conventional approach ceases to provide true representation of physical reality. In order to represent the effect of the microstress variation through the unit cell and properly capture the meaningful macroscopic steep stress gradient fields, one must retain the volume average of the microstress distribution as the ‘stress’ acting on the cell but also the higher-order effects of the microstress distribution on the element. One of the higher-order effects of the microstress distribution is the set of first moments of microtractions, which provides couples on the surface of the cell. In a recent study of modeling the effective moduli of debonded interface by the PI, it was found from micromechanics that the stresses on the boundary of the cell lead to resultant forces and moments, as in micropolar (couple stress) theory. The couple stresses are conjugate to gradients of local rotation. Thus, in the elastic couple stress theory, the couple stresses are proportional to local rotation gradients, which are themselves proportional to differences of gradients of strain. This also results in the introduction of material lengths into the constitutive relations for dimensional consistency. Hence, the effect of absolute size of the microstructure will be incorporated in the constitutive description. The presence of the length parameter, in turn, implies that the micropolar theory encompasses the size effects that are ignored in the classical anisotropic elasticity theory.

A higher-order continuum theory such as micropolar theory may provide a significant improvement in analyzing the stress behavior of composite structures near the steep stress gradient zone, and further predicting the microstress near this region where the failure may initiate in this microscale. Therefore, there is a need to implement micropolar theory into the ply level in the laminate analysis. Firstly, emphasis is placed on deriving micropolar composite moduli and assessing the singular behavior of stresses in the regions close to the exposed free edge. A finite element technique to derive these moduli is presented. The effects of micropolar theory on the normal stresses along the "artificial" interface that is an artifact of ply homogenization, particularly near the high macrostress gradient region, are also examined. Secondly, the microstress along the fiber-matrix interface of the 'critical' cell are of interest. 'Critical' cell is defined as the cell on the interface of matrix and composite and near the free edge of the lamina, where the high macrostress gradient is found due to material and/or geometric discontinuity.

A finite element approach to calculate micropolar moduli in orthotropic solids is presented. A square fibrous unit cell is employed in the analysis. The application of classical elasticity theory and micropolar theory in predicting the microstress fields from macrostress fields near the high macro-gradient zone of the free edge problem in composite laminates will be presented in detail. The composite consist of Sigma 1240 (silicon carbide) fibers (Young's modulus: 325 GPa and Poisson's ratio: 0.15) and epoxy matrix (Young's modulus: 3.45 GPa and Poisson' ratio: 0.35). A composite laminate is used to critically examine and compare the stress solutions from these two theories with "exact" solutions. 30.7% V_f fibrous unit cells are utilized to construct the composite laminate model shown in Fig. 2.

In order to assess if the effective modulus theory represents reasonable stress field predictions of the micromechanics model, the comparison of the resultant stresses around the boundary of the critical cell is evaluated and listed in Table 1. A strong indication of the improved stress predictions from the MP model is demonstrated. Notice that the resultant shear stress is anti-symmetric, hence, the unit cell is now subjected to both resultant stresses and moments. The total moment from MP model is computed by the combination of moment resulting from the normal stresses and couple stress of micropolar theory. Overall, good agreement is achieved between the MM and MP models. While the EM and MP models may produce irregularity in the stress field prediction, the MP resultant stresses compare quite well with those given by the "exact" analysis (MM model). After evaluating the boundary of the critical cell, one can conclude that the micropolar theory significantly improves the prediction of resultant stresses near the free edge of the composite laminate.

The micromechanics model (MM) which models the fibers explicitly in the finite element method will serve as "exact" solutions for the laminates within the bounds of the FEM analysis. The stress fields based on effective modulus model (EM) from classical elasticity theory and micropolar model (MP) from micropolar theory are evaluated and compared with the "exact" solutions. Note that in the composite the ply interfaces are truly matrix material, but the effective modulus representation (EM and MP models) leads to artificial results – caused by the "discontinuity" in moduli at the interface in the model. The "layered" composites create a high macrostress gradient near the free edge. The only way to improve the results is to represent the microstructure explicitly (MM model). Also in the MP model, the couple stress traction vector must vanish on the interface with a classical epoxy matrix. Special attention is focused on the microstress along fiber/matrix interface of the critical cell near the high macrostress gradient region. These microstresses are crucial since failure of the composites most likely will initiate along the fiber/matrix interface. It has been demonstrated that the effective modulus model (EM) is not able to capture these microstresses accurately by the PI. The proposed micropolar theory (MP), which includes a couple stress and an independent rotation in addition to the conventional stresses and displacements of elasticity theory, respectively, may predict these microstresses precisely.

Micromechanical stresses affect the strength of fiber reinforced composites. In addition, initial cracking in composites usually occurs in the matrix or the interface between fiber and matrix. Therefore, the most important part in the design analysis of composite lamina, especially in the failure analysis of composites is the stress distribution along fiber/matrix interface. For the present boundary value problem, the implementation of micropolar theory into composite laminate mechanics appears to be beneficial in predicting these microstress. To demonstrate this point, nodal forces attained from the boundary of the critical cell are applied to a unit cell. For MP model, in addition to the direct nodal forces, the nodal force due to the couple stress is also implemented to the computation scheme around the boundary of the critical cell. The microstress from MM, EM and MP models are then compared.

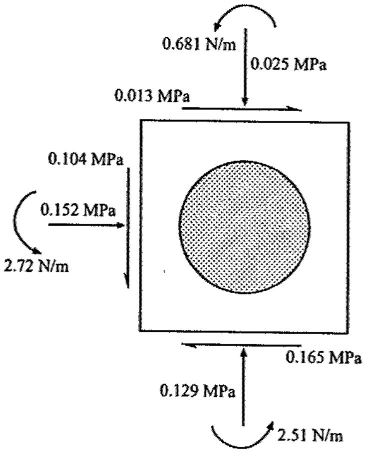
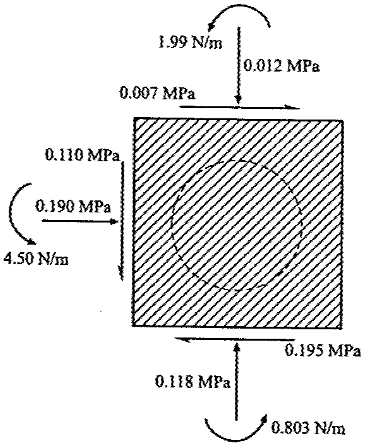
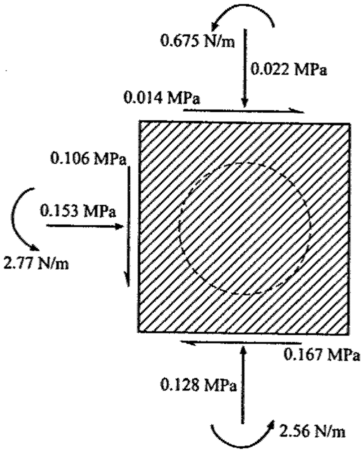
The microstress prediction of the first case obtained from traction boundary conditions are plotted in Figs. 3(a-d). The solid lines represent MM microstress. In the solid curves of Figs. 3(a, d), the distribution of σ_r and $\sigma_{r\theta}$, which, of course are equal in exact elasticity solution but are natural boundary conditions in the FEM. Hence, the proximity of the results (the solid lines are actually two curves) is a sign of the convergence of the FEM solution. In Fig. 3(c), the matrix stress distribution of σ_θ is displayed. The microstress σ_θ in the fiber are also presented in Fig. 3(b). The other curves in Figs. 3(a-d) represent EM and MP models. In Figs. 3(a-d), the EM and MP results are plotted in open diamond and solid circles, respectively. The microstress from traction boundary conditions calculated from EM and MP models along the three critical cell boundaries, $y_o = h/2, -h/2$ and $x_o = -h/2$, and traction free boundary at $x_o = h/2$, where x_o, y_o are the center coordinate of the critical fiber, are displayed and compared with the exact MM model. It is shown in Figs. 3(a-d) that the microstress from the MP model is in very good agreement with the "exact" microstress. Fig. 4 shows that micropolar theory is able to improve greatly the prediction of strain distribution, ε_y, at the free edge of the critical cell.

CONCLUSIONS

The micropolar homogenization is used to predict the microstress distribution in the region of high macrostress gradient of the composite laminates. The in-plane shear moduli and the bending moduli are determined from a nine-cell model and a long strip of unit cells respectively. In order to substantiate its applicability, a composite laminate with free edge under uniform axial strain have been studied. The following conclusions may be drawn:

1. The micropolar homogenization method is introduced to determine the effective moduli of composite materials by means of the finite element method. In addition to the classical effective moduli, the micropolar shear and bending moduli are utilized to introduce the cell size factor that exists in micropolar theory.
2. In the classical elasticity theory, the fiber volume fraction and the cell size affect the stress response of the composite laminate. First, in the class of problems studied there is inconsistency in predicting the normal stress, especially at the free edge when 30.7% V_f cell laminates are employed. The EM model gives a distortion of physics since the singular stress is tensile at the free edge while the MM stress is compressive. Second, a strong indication of a 'micro-zone of influence' around the boundary of the cell near the free edge is observed. The term 'micro-zone of influence' implies that the stress and strain distributions around the boundary of the cell vary with the cell size (fiber size). A 'Micro-zone of influence' can also be interpreted as the influence of a particular fiber is only felt within a region of fiber size (dimension h). Due to the importance of the cell size on predicting the elastic response of composite laminates, the micropolar theory which takes into account the cell size or dimension is studied.
3. Similar to the classical elasticity theory, the application of micropolar theory to composite laminate introduces artificial interfaces leading to severe macrostress gradient, which can distort the physics of the problem by reversing the sign of the normal stress near the free edge region. The inconsistency in predicting the normal stress at the artificial interface implies that the effective moduli approach, the classical and micropolar elasticity theory, needs careful interpretation with regard to the prediction of physical behavior in the present problem, as well as in other problems in which effective singularities exist. The advantage of the micropolar theory can be clearly seen by evaluating the resultant stresses on the boundary of the critical cell, near the free edge of the composite laminate. It is clear that the classical effective modulus theory (EM model) is not able to predict these stresses, while the micropolar theory produces accurate prediction of the resultant stresses.
4. The microstress predictions near the steep macrostress gradient using micropolar theory from the ply level for all cases are very promising although the micropolar theory only considers the gradient of the normal stress (couple stress) but not shear stress. These stresses are responsible the failure initiation process in composites since the composite failure always originates from the microscale. In general, the micropolar theory improves the microstress predictions using both displacement and traction boundary conditions imposed on the critical cell boundaries. However, the use of displacement boundary conditions in the laminate with higher fiber volume fraction, such as in the second case, is not able to capture or even provide similar microstress trends as in the "exact" solutions (MM model). Note that the independent rotation has not been taken into account in the displacement boundary conditions along the cell boundary. It is hopeful that the inclusion of this rotation in the boundary condition will further improve the microstress prediction.

Table 1: Resultant stresses on the 'critical' cell

MM (Micromechanics Model)	
EM (Effective Modulus Model)	
MP (Micropolar Model)	

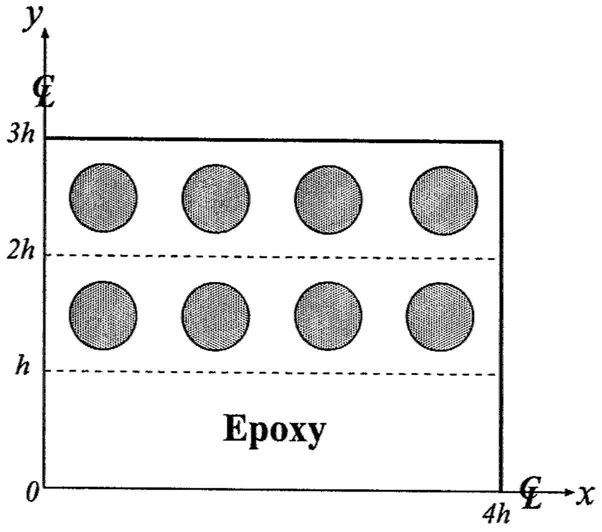


Fig. 2 2-row composite lamina with fiber diameter: 100 μm and cell size: 160 μm × 160 μm ($V_f = 30.7\%$)

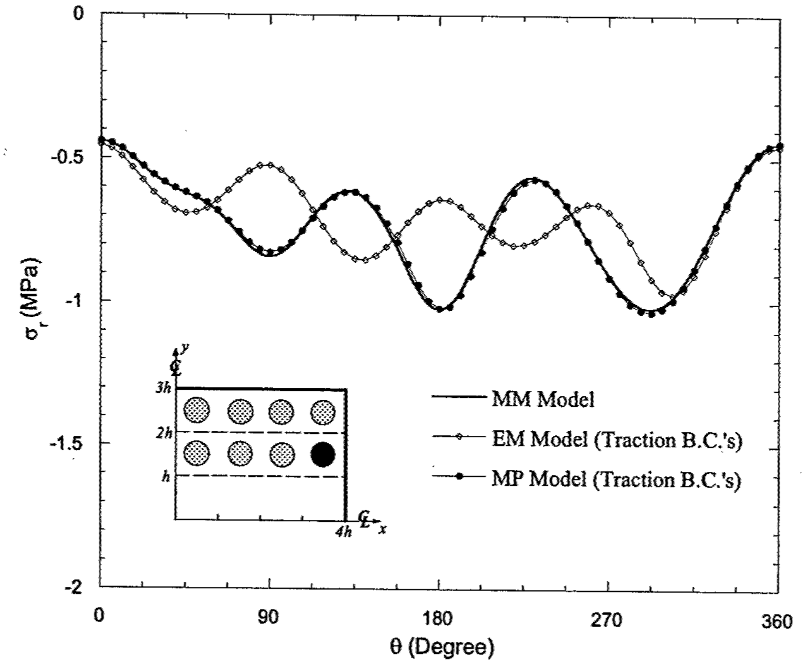


Fig. 3(a) Case 1: σ_r of the critical cell along the fiber/matrix interface

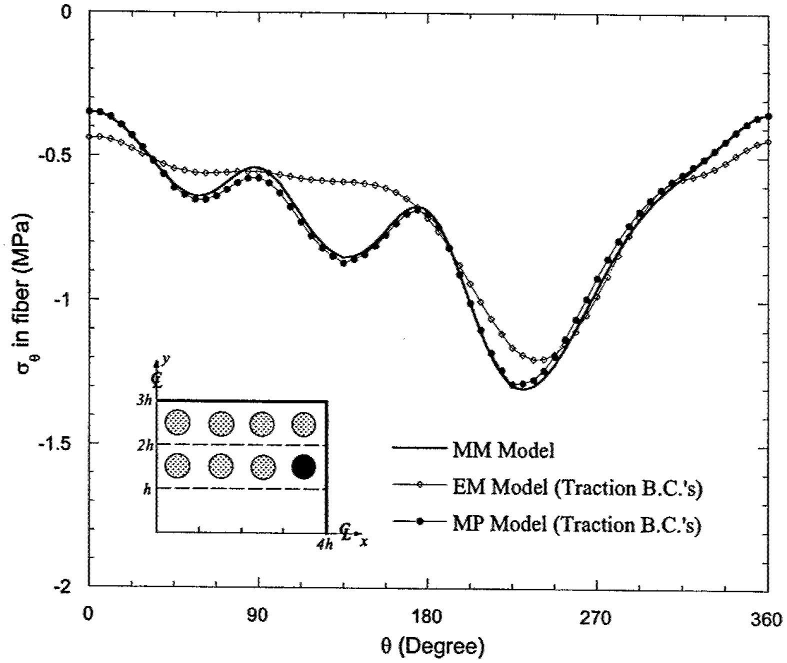


Fig. 3(b) Case 1: σ_θ in the fiber of the critical cell along the fiber/matrix interface

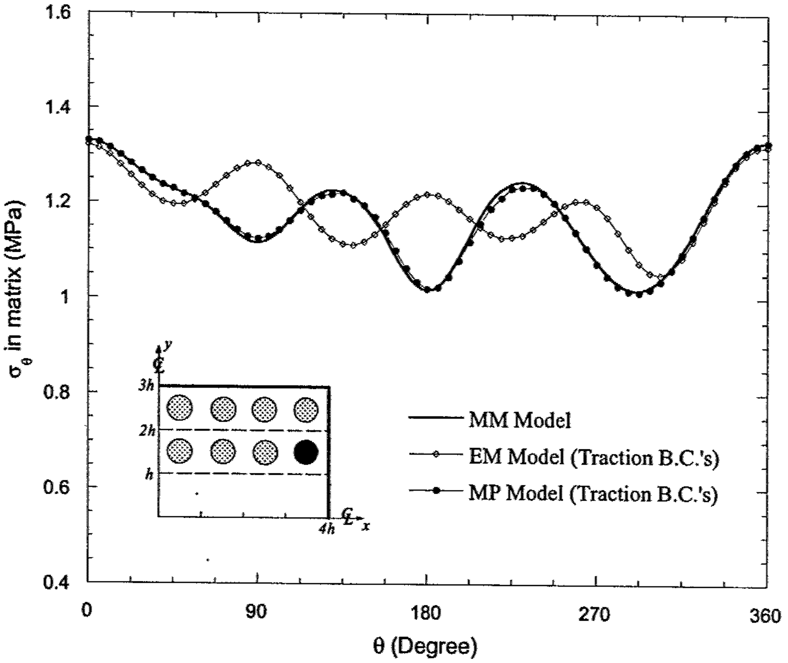


Fig. 3(c) Case 1: σ_θ in the matrix of the critical cell along the fiber/matrix interface

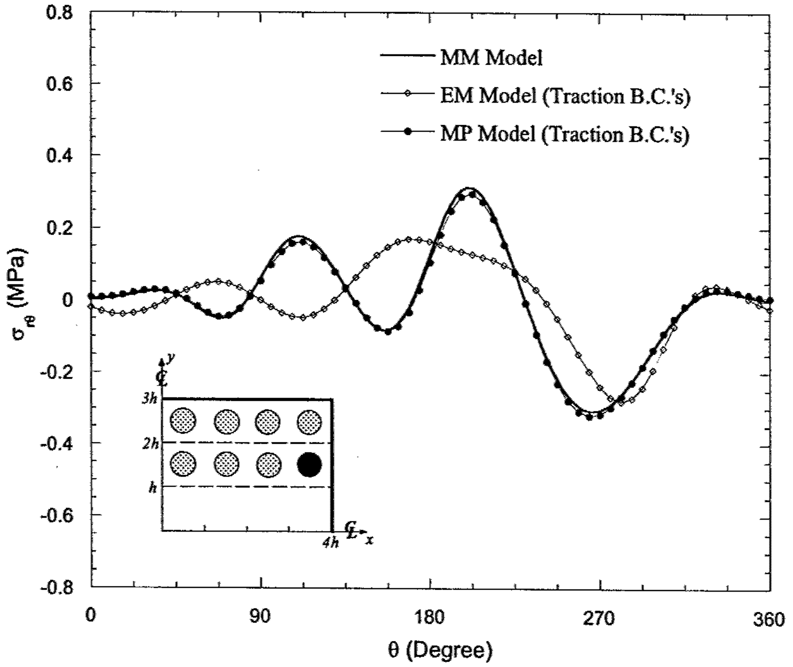


Fig. 3(d) Case 1: $\sigma_{r\theta}$ of the critical cell along the fiber/matrix interface

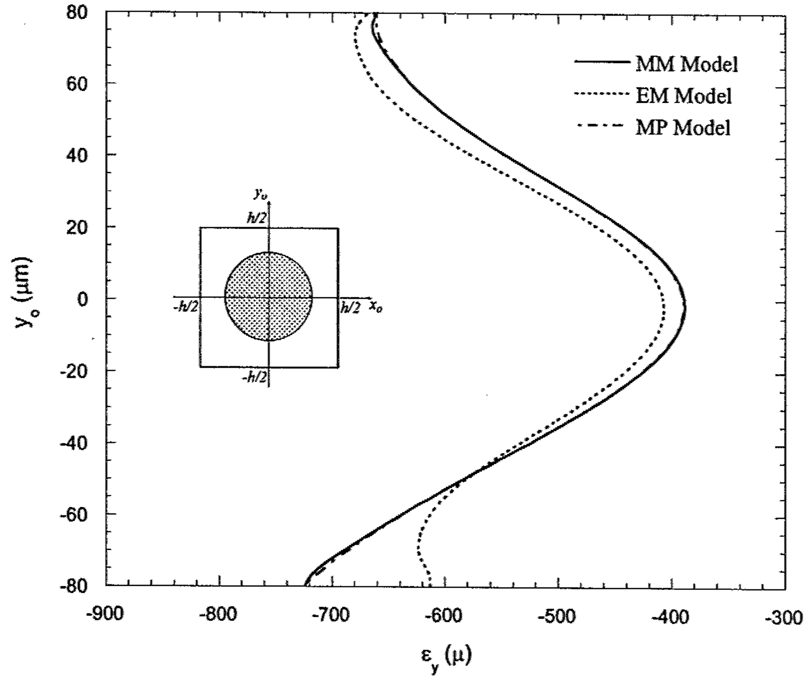


Fig. 4 Case 1: ε_y of the critical cell along $x_o = h/2$