Published Online on 29 June 2016

Proc Indian Natn Sci Acad **82** No. 2 June Spl Issue 2016 pp. 173-181

DOI: 10.16943/ptinsa/2016/48411

Research Paper

Multiscale Modeling of Failure in Composite Materials

RAMESH TALREJA*
Department of Aerospace Engineering, Department of Materials Science and Engineering, Texas A&M University, College Station, Texas 77843, USA
Department of Engineering Science and Mathematics, Luleå University of Technology, 971 87 Luleå, Sweden

(Received on 20 April 2016; Accepted on 27 April 2016)

Failure in composite materials is known to initiate at the level of constituents. Further development of the failure process and ultimate failure of the composite structure depend on the fiber architecture and other geometrical details. A composite failure analysis must therefore be at multiple length scales. This paper will outline a multiscale modeling scheme and illustrate the approach with two examples: tensile fiber failure and transverse matrix cracking. For the case of fiber failure, a five-cylinder axisymmetric finite element model containing an initially broken fiber at the center will be used to conduct stress analysis and formation of a failure plane will be simulated by a crack growth procedure. The transverse crack formation will be analyzed as a linking up of fiber-matrix debond cracks. Formation of these cracks will in turn be analyzed by an energy-based criterion. The local scale modeling will take account of the manufacturing induced irregularities and defects by appropriate representation of these in the failure analysis. Finally, an assessment of the multiscale approach as a rational alternative to the currently used failure theories, which are formulated on homogenized composites, will be presented and the challenges remaining to address in future will be outlined.

Keywords: Composite Failure; Multiscale Modeling; Failure Theories

Introduction

Multiscale modeling is a fertile field today with a flurry of contributions. However, closer examination of the literature indicates that most of the concepts and approaches in multiscale modeling are motivated by experience with metals. Composite material failure has its characteristics quite different from metallic failure and a proper approach to addressing it should account for those. This paper will briefly describe the observed mechanisms of failure in unidirectional composites in basic loading modes and outline the rich and intricate features of the failure events in composite laminates. Then, keeping the physical nature of composite failure in view, the role of manufacturing defects will be discussed. This will serve to clarify the necessity of addressing composite failure on its own merit rather than adapting the metal-based approaches to this field. A methodology for this purpose will be proposed. There is a good deal of progress made to develop the methodology, but challenges remain. Those challenges will be outlined after illustrating the recent work on a couple of failure modes: failure in axial tension, and in transverse tension, of unidirectional composites.

Failure Mechanisms in Unidirectional Composites

It is convenient to address these mechanisms with respect to the elementary loading modes, viz., tension along fibers, compression along fibers, tension across fibers, compression across fibers, and in-plane shear. The following will briefly describe failure mechanisms observed in each case, leaving details to the cited references.

Tension Along Fibers

Fiber failure in a unidirectional composite under imposed overall axial tension has been studied extensively. A recent work using high resolution X-

**Author for Correspondence: E-mail: talreja@tamu.edu*

ray micro-tomography (Aroush *et al*., 2006) provides clear evidence of the statistical nature of this process (Fig. 1). As reported in that work, fiber breaks appear initially at low loads as single failures at discrete locations because of failures at weak points. On increasing the applied load, more fibers fail, mostly near the previously broken fibers, and the so-called doublets form. This process continues until one or more of the broken fiber clusters grow unstably to failure of the composite.

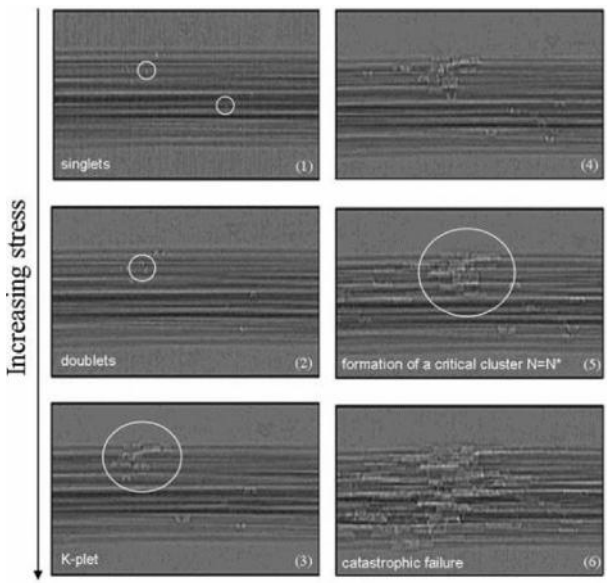


Fig. 1. Sequence of fiber failures in a unidirectional composite under axial tension (Aroush *et al.*, 2006)

Compression Along Fibers

As described by Jelf and Fleck (1992), the fiber failure in compression may be categorized as elastic microbuckling or plastic microbuckling, depending on whether the matrix stress-strain behavior is linear or non-linear. For the latter case, kink bands govern the compressive strength and fiber misalignment and matrix shear yielding are found to be important parameters (Kyriakidis *et al.*, 1995). These authors found that in the presence of fiber waviness, localization of shear deformation occurs in the matrix. This forms bands and the flow of the matrix in the bands results in bending of fibers and eventual breakage. Fig. 2 illustrates schematically the early stage of microbuckling leading to formation of a kink band (Berbinau *et al.*, 1999).

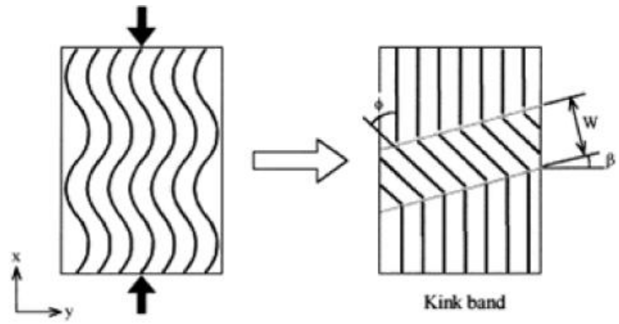
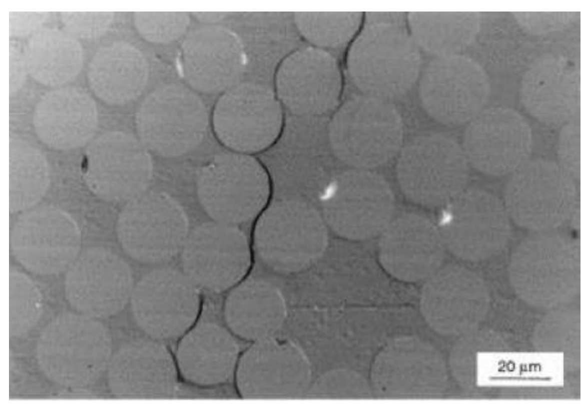


Fig. 2. Schematic illustration of fiber microbuckling and kink band formation in a unidirectional composite subjected to axial compression (Berbinau *et al.*, 1999)

Tension Across Fibers

On loading a unidirectional composite under tension normal to fibers, failure occurs suddenly and at low stress levels. The mechanisms leading to the catastrophic failure are conveniently studied by observing the initiation and progression of cracks within the plies of a laminate. The appearance of these cracks is typified by the images shown in Fig. 3 (Gamstedt and Sjögren, 1999).



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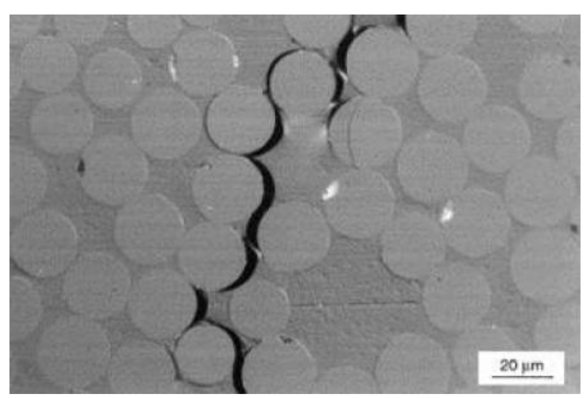

B

Fig. 3. From Gamstedt and Sjögren, 1999

Compression across fibers. When compression is applied normal to the fibers, the failure is found to occur along a plane that is inclined to the loading direction, as reported in González and LLorca (2007) (Fig. 4). On closer examination, it was found that microscopic cracks formed due to shear and the coalescence of these cracks led to failure along the inclined plane.

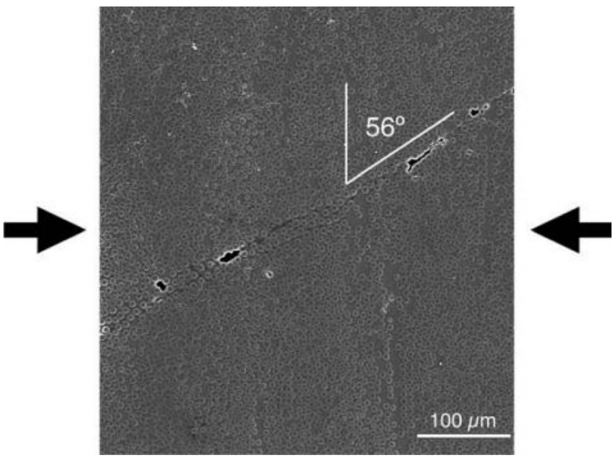

Fig. 4. From González and LLorca (2007)

In-plane shear. Under an in-plane shear stress a unidirectional composite displays nonlinear behavior. A part of this is due to a shear-induced flow of the matrix and the other part is caused by cracks formed in the matrix. Such cracks are illustrated in the image shown in Fig. 5 (Redon, 2000). These cracks, as shown in the figure, form as multiple cracks with their planes inclined to the fiber axis. On increased loading, the cracks turn along the fibers and merge together, forming a failure plane. Such a failure plane is also formed under compression normal to fibers (Fig. 4), indicating the role of the shear stress on the plane.

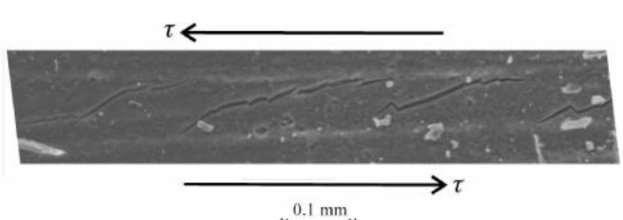

Fig. 5. Shear failure (From Redon, 2000)

Multiscale Modeling

Failure theories developed on homogeneous composites have not succeeded (Soden *et al.*, 1998) for the simple reason that it is not possible to incorporate failure mechanisms in the models without conducting stress analysis at the constituent scale where failure events occur. Also, the diverse failure modes summarized above require that each of these modes be analyzed using their driving forces acting at the local levels. This consideration leads naturally to the need for multiscale modeling of failure. However, it must be realized that the scales in such a modeling approach must follow the governing scales of failure that are not necessarily the geometrical scales of the microstructural and architectural hierarchy of the composite. To illustrate this point, note that the tensile failure (Fig. 1) and compressive failure (Fig. 2) of a unidirectional composite display very different governing length scales. While the tensile failure initiates at the scale of fiber diameter, the initiation of compressive failure is triggered by microbuckling, which has a wavelength depending on the fiber misalignment. Similarly, the tensile and compressive failures of a unidirectional composite under transverse loading have different governing scales. The in-plane shear failure of a unidirectional composite is often mistakenly attributed to decohesion along an inclined plane, while closer examination of the failure plane indicates that the initiation of this failure lies in formation of submicroscopic cracks between fibers (Fig. 5).

After the early failure events have occurred in a unidirectional composite in different remotely applied loading modes, their progression is governed by the local conditions. These local conditions may be expressed as driving forces, which come from energy supplied by the material surrounding the failing elements. The size-scale of the failed elements (often cracks) determines the characteristic scale of the surrounding medium that participates in the energy exchange.

In a composite laminate, the unidirectional composite acts as a building block in the form of layers stacked in different orientations. Under a general loading imposed on the laminate, the individual layers are subjected to in-plane stresses that can be expressed in the material coordinate system of the layer as normal stresses along fibers and across fibers and the in-plane shear stress (Fig. 5). Under these stresses, the progression of the failure events culminates in formation of a crack or a failure plane. At that point, the laminate itself remains intact, unless the failure mode is tensile failure of fibers. Naming this as critical failure, the subcritical failure mechanisms consist of a range of multiple cracking modes illustrated in Fig. 6. Details of the observed images like these show that the scales of failure evolve at different stages of the failure process.

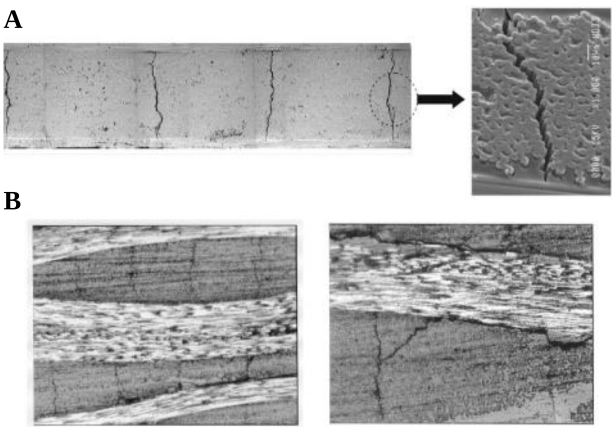

Fig. 6. Multiple cracking in a laminate (A) and in a woven fabric composite (B)

In the following, the failure analysis will be illustrated for two selected failure modes in unidirectional composites: axial tensile failure (Fig. 1) and transverse tensile failure (Fig. 3). Following that, the subcritical failure analysis for laminates will be discussed. An overall scheme for composite failure analysis will be outlined in which its connection with manufacturing defects will be incorporated.

Axial Tensile Failure of Unidirectional Composites

As illustrated in Fig. 1, the axial tensile failure of a unidirectional composite is a stochastic process. At the root of this process is the fiber failure itself, which is a random process governed by the randomly distributed defects along the fiber length. Based on the weak-link theory, Weibull distribution captures the probability of fiber failure well. When the fibers are embedded in the matrix, the progression of failure from one fiber to the next becomes another random process. As illustrated by Fig. 1, the fibers fail at discrete locations initially, and these failures are described as singlets. The presence of a fiber failure enhances stresses in the neighboring fibers and, depending on the distribution of the defects (weak points) in these fibers, next fiber failure ensues. The formation of "doublets" and "k-plets", k being an integer, occurs in a random manner. Experimental observations have indicated that in brittle composites such as glass-epoxy and carbon-epoxy, final failure ensues from unstable growth of a plane connecting a cluster of failed fibers. Previous analyses have focused on determining enhancement of the failure probability in a fiber cluster with one (central) fiber already broken (Nedele and Wisnom, 1994). Figure 7 illustrates the axisymmetric model used in Nedele and Wisnom (1994) for finite-element based stress analysis. As shown in the cross-sectional image (Fig. 7, upper left), a broken fiber is assumed to be surrounded by hexagonally arranged six intact fibers. In the model (Fig. 7, upper right), the intact fibers are smeared together and represented by a cylinder (ring in the cross-section). Two cylinders – one inner and the other outer – bound this cylinder with their cross sections such that the fiber volume fraction in the composite is represented. Finally, a homogenized composite cylinder is placed as an outer cylinder in the five-cylinder assembly to represent the composite in which the localized fiber failure process is taking place. Figure 7 (lower) illustrates the axial section of the five-cylinder assembly subjected to axial tension.

Nedele and Wisnom (1994) considered the stress concentration caused by the broken fiber on the surrounding intact fibers without accounting for failure of the matrix. In a yet unpublished work, Zhuang *et al.* (2016) have analyzed matrix cracking emanating from the broken fiber and its effect on stress concentration on the neighboring fibers as well as the ensuing enhancement of the failure probability. This failure probability was found to be highest over a small length of the intact fibers at the intersection of the matrix cracks and the fibers. The enhancement in this failure probability was found to be significantly higher than that calculated without considering the matrix crack. Zhuang *et al.* (2016) considered also the effect of fiber-matrix debonding on the matrix cracking.

Transverse Tensile Failure of Unidirectional Composites

It is important to recognize that in the absence of a crack, or a weak plane that can potentially form a crack, failure in a given material will be a "point process", i.e. it will initiate at a material point when

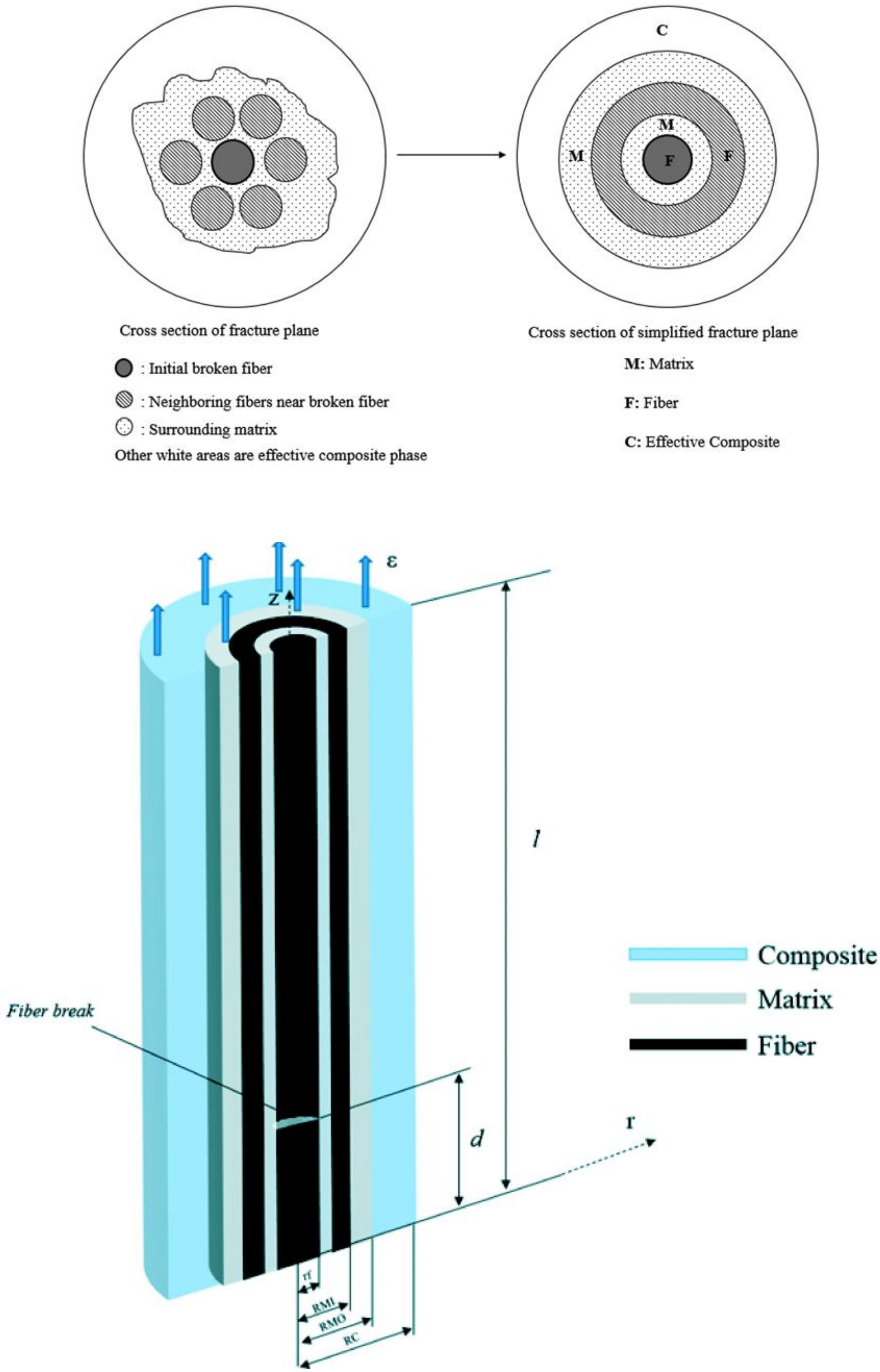

Fig. 7. The five-cylinder axisymmetric model for analysis of local failure from an initially broken fiber

critical conditions for the particular failure mode are met at that point. Subsequent events will depend on the region in which the failed material point exists. If the material point lies in a brittle region, which has little capacity to deform in-elastically (i.e., irreversibly), then the consequence of failure can be formation of a brittle crack, if appropriate conditions exist, such as a critical release of energy along a preferred plane. On the other hand, if the region is a polymer that deforms in-elastically, then crazes or shear bands, or both, can form (Donald and Kramer, 1982), leading eventually to ductile failure.

Before examining whether the failure ensued is to be brittle or ductile, it is appropriate to look at the stress field under which failure initiates. It is a common error to assume that a polymer that shows extensive inelastic deformation under a uniaxial test in the laboratory also behaves in-elastically within a composite with stiff reinforcement. Asp *et al.* (1996a,b) found that the behavior of an epoxy polymer subjected to the so-called "composite like" stress state was brittle, in spite of extensive ductility displayed under uniaxial stress. This gave a plausible explanation of the observed low strain to failure under transverse tension of unidirectional composites and the insensitivity of this strain to modifications of the polymer morphology.

According to Asp *et al.* (1996a,b), in regions of matrix close to the stiff fibres within a unidirectional composite, the stress state developed under remote transverse tension is tri-axial with nearly equal principal stresses. Independent tests conducted on an epoxy polymer produced critical value of the dilatational energy density, which when used for the same epoxy within the composite, predicted the composite failure stress well. The observed mechanism in the unreinforced polymer under hydrostatic tension was cavitation and it was reasonable to assume that the expansion of the cavity formed becomes unstable at a material-specific value associated with the initiation of the instability.

A remarkable implication of the theory advanced in Asp *et al.* (1996a,b) is that what is commonly assumed to be fiber-matrix de-bonding may actually be a consequence of the brittle failure induced by the cavity "burst" when the critical dilatational energy density is reached. Since this happens close to the fiber surface (at specific locations), where the largest dilatational energy density exists, the consequent fiber-matrix interface breakage appears as debonding.

The fiber-matrix debonding mechanism is also possible without the matrix cavitation failure as a precursor. This will be the case if favorable conditions for cavitation do not exist or if the fiber-matrix interface is sufficiently weak or is sufficiently weakened by defects. In that case, the radial tensile stress, and possibly this stress combined with the shear stress on the fiber surface, will break the fiber-matrix interface bonds, initiating de-bonding. For modeling purposes, it is difficult to know what interface failure properties to use, as these depend on the actual quality of the bond formed during the composite manufacturing process, which is not the same for model composites with one or few filaments that are used for experimental determination of the bond characteristics. The interface bond strength cannot be determined accurately by theoretical means. Several experimental methods have therefore been devised (see Zhandarov and Mader, 2005 for a review). These are either stress-based (strength) or energy-based (toughness) methods. As noted above, the characteristics of the fiber-matrix interface obtained by the experimental methods are commonly under simple conditions (e.g. single-fiber tests). Using the material constants thus obtained for interfaces that are under constrained conditions within composites would require caution. Also, applying the interface toughness criterion for evaluating initiation of fiber-matrix debonding faces difficulties due to the uncertainty of knowing the flaw size and its variability.

For ductile failure to occur under transverse tension of a UD composite, conditions must exist for inelastic deformation of the polymer matrix within the composite. Since the inelastic deformation requires shear stress to drive it, the distortional part of the strain energy density at a point must be sufficient to initiate what may be called "yielding" (although this term originates from crystalline metals behavior). For isotropic metals, the initiation of yielding is satisfactorily given by the critical value of the distortional energy density obtained experimentally for the given metal. Equivalently, the yield criterion for metals can be expressed in terms of the second invariant of the deviatoric stress tensor, as is the case for the von Mises criterion. The initiation of yielding in polymers is governed by molecular phenomena that differ significantly from the dislocation motion underlying yielding of crystalline metals. Still, it is common to describe the onset of inelastic deformation in polymers by the approaches used for metal yielding. In contrast to metals, the inelastic response of glassy polymers displays pressure sensitivity, as discussed by Rottler and Robbins (2001). This has prompted modifying the metal yield criteria by including the hydrostatic stress, e.g. by adding to the threshold of the octahedral shear stress t_0 a constant a times the mean pressure p, as

$$\tau^{y}_{oct} = \tau_0 \qquad p \tag{1}$$

where p is the average of the three principal stresses, $p = -(\sigma_1 + \sigma_2 + \sigma_3)/3$.

Equation (1) is the modified von Mises yield criterion, which in energy terms states that the dilatational energy density contributes as well to the shear-driven onset of inelastic deformation in polymers. Additionally, temperature and strain rate are also found to affect the inelastic deformation (Arruda *et al.*, 1995).

In a polymer matrix within a unidirectional composite, the stress tri-axiality is generally high except in resin-rich regions. The inelastic deformation will thus tend to occur away from the fiber-matrix interfaces. Once initiated, the inelastic deformation can lead to shear banding before crack formation. Estevez *et al.* (2000) have studied the crack formation process in glassy polymers by considering the competition between shear banding and crazing. Based on their study it can be stated that the role of the distortional part of the strain energy density at a point is to localize inelastic deformation in shear bands, while the dilatational component is responsible for cavitation leading to craze formation, craze widening and breakdown of craze fibrils. The mix of the two energy components determines the ease or difficulty of ductile crack formation in the matrix within the composite.

Failure in Composite Laminates

As described above, unidirectional composites form the building blocks in many composite structures, e.g. in stacked configurations in multidirectional laminates. Failure ensued in a single layer is often the beginning and not the end of the structural failure. In going beyond the unidirectional composite failure, two aspects are noteworthy: one, that the unidirectional composite failure within a layer is necessarily under combined loading, and two, that this failure is constrained by the presence of the other differently oriented layers. When failure in a unidirectional composite lying within a laminate occurs, it is not an ultimate failure in the sense of breaking apart as separate pieces, but rather as initiation of a crack that has its plane aligned with the fibre direction in the composite layer. This failure, described in the early literature as "first-ply failure", has a progression consisting of multiple parallel cracks (see Fig. 6), which increase in number, reducing their mutual spacing, until a saturation state is reached. Failure in other plies progresses similarly, in a sequence determined by the criticality of their stress states.

The schematic illustration of subcritical damage in a cross-ply laminate in Fig. 8 brings out the complexity of failure events. The force-displacement response shown to the right in the figure illustrates the challenges involved in treating the interconnected cracks in multiple planes. It is clear that only a multiscale approach will be able to deal with such situations. It is also clear from this relatively simple failure scenario (compared to more complex composite architecture) that the characteristic scales

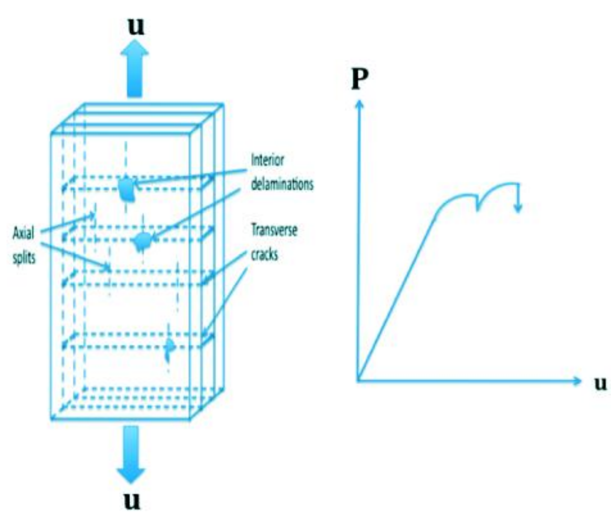

Fig. 8. Schematic illustration of multiple transverse cracking, axial splits and interior delamination as subcritical mechanisms in a cross-ply composite laminate. The load-displacement response under prescribed displacement is illustrated to the right

of failure events evolve with different hierarchy than what is in the microstructure and architecture of the composite. The composite laminate response for the case of distributed multiple cracking in multiple orientations has been successfully treated by damage mechanics approaches (Talreja and Singh, 2012). However, the final failure event leading to ultimate failure of a multidirectional composite laminate still remains a challenge.

Additional challenges in composite failure modeling lie in accounting for defects induced by manufacturing. An integral approach to defects and damage should account for failure events (e.g. microcracks) and manufacturing defects (e.g. matrix voids and disbonds between layers) by describing a "real" initial material state (RIMS). A proper concept for characterization of RIMS is the representative volume element (RVE). The following discussion proposes the future direction in which failure assessment of composites needs to go as an alternative to the current failure theories based on homogenization of the microstructure.

Future Direction in Composite Failure Analysis

A roadmap for an integral multiscale approach to composite failure is shown in Fig. 9. As indicated there, the first step is to characterize the microstructure of the composite as it results from the manufacturing process used. The characterization of the microstructure is to be at a scale needed for the failure analysis. Thus, depending on which failure mode is being analyzed, e.g. a fiber failure mode in a unidirectional composite, the choice of the micro-structural region will be accordingly. In each case, the micro-structural region must also include the appropriate manufacturing defects (e.g. voids and broken fibers) within the region. This RIMS in this region is labeled as RVE-1. The stress and failure analysis of this RVE will generate the conditions (criteria) for the operating failure mode. The failure conditions for lamina failure modes will enter the analyses of the subsequent failure modes in a laminate via appropriate RVE-2.

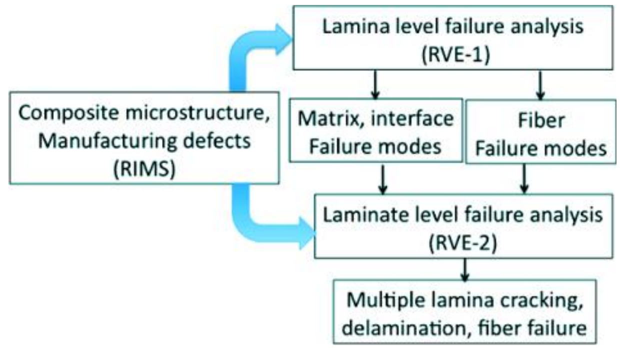

Fig. 9: A roadmap for failure analysis of composite laminates

Concluding Remarks

This paper has illustrated the complexity involved in failure of composite laminates by showing key images for each of the basic mechanisms observed in unidirectional composites. The failure events in a composite laminates evolve with different characteristics and have been successfully treated in the field described as damage mechanics. However, damage mechanics deals only with the composite laminate response to distributed multiple cracking. The path from the subcritical failure events, as the distributed damage is described, to the ultimate composite failure still remains a challenge.

An integral multiscale failure analysis roadmap has been outlined here. Hurdles in the roadmap are mainly in treating intralaminar cracks that have diverted into the lamina interfaces, and the interconnection between these cracks that results from growth in the interfaces. The load bearing capacity of a laminate with this type of damage is yet to be determined reliably. Current trends in treating this problem by the cohesive zone models are subject to uncertainty due to the non-uniqueness of the material parameters (strength and fracture toughness) entering such models.

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