

Multiaxial and Multiscale Implications of Dissipative Behavior of Composites

**J.G. Michopoulos^{a1}, A.P. Iliopoulos^a, J.C. Steuben^a,
J.C. Hermanson^b**

^a U.S. Naval Research Laboratory, Computational Multiphysics System Lab., Code 6394,
Washington DC, 20375, USA

^b U.S. Forest Products Lab., Madison WI, 53726, USA

Abstract. A brief description of the progress on mechatronic multi-degree of freedom material testers developed at the US Naval Research Laboratory (US-NRL) is given to describe the enabling technology for acquiring data that encapsulate both the recoverable and the dissipative behaviors of various composite material systems under quasi-static multiaxial loading conditions. The notion of material equivalence is then explored from the perspective of the data-driven dissipative behavior of multiaxially tested composite laminates. Emphasis is given by considering the same fiber within the same resins and vice versa. The effect of different curing conditions is also examined. As a follow-up, an overview of a multiscale computational framework is also outlined for the purpose of introducing multiscale implications of how macro-scale behavior in terms of experimental data can yield information about the behavior of materials at lower length scales.

1. Introduction

Contemporary cradle-to-grave engineering requirements placed on system products include safety, economy, maximum functionality, manufacturability, and maintainability. Combined with the need for qualification, certification, and utilization of such systems, these requirements have significantly raised the demand for validated, efficient, and rapid simulation of the behavior of complex whole systems. In the particularly complex category of material and structural systems known as Polymer Matrix Composites (PMCs), which exhibit a time-varying degradation behavior over large time scales where aging and maintenance are critical, life extension for usability purposes has become a focal area of interest. On the other hand, simulations inherit all of their utility and economic properties from those of the analytical and computational models they are based upon. Data-driven determination of analytical and computational models is an activity that contributes to the objectives mentioned previously by promoting the embedding of validated realism originating from the measured behavioral characteristics of PMCs encoded in the systematically collected data.

In an effort to be consistent with this view, our team at the U.S. Naval Research Laboratory (US-NRL) has developed a system identification approach utilizing custom-made robotic testing machines. These machines possess the unique capability to expose material specimens to loading paths spanning the representative loading space of the specimen structure in order to achieve

¹ corresponding author



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data-driven characterization of the constitutive response of PMC systems. A short history of the multi-decade evolution of multi-degree of freedom robotic testing machines is given elsewhere [1, 2, 3].

The motivating goals of the work presented herein are two-fold. First, to demonstrate that if structural response of composites is recorded in terms of their exposure to multi-axial loading in a manner that accounts for their dissipative behavior due to strain-induced damage, then comparing materials and designing composite structures may require a more enriched approach than the one followed currently in many industrial applications by the relevant stakeholders. It should be noted here that other investigators have focused their attention towards the dissipative aspects of PMCs such as [4, 5, 6, 7, 8, 9], but none approaches the topic from the perspective of multiaxiality of loading and strain induced damage as it will be described here.

The second motivating goal is to demonstrate some of the opportunities and difficulties in inferring the micro-scale behavior of constituent materials from both the conservative and non-conservative perspectives, when experimental data are available at the macro-scale of actual composite parts.

2. Overview of NRL's Multiaxial Loading Systems

To apply multiaxial loading conditions on PMC coupons with the purpose of identifying the bulk lamina constitutive characteristics both in terms of their elastic and inelastic responses, our group has embarked in an effort of prototyping and using custom made multi-degree of freedom (m-DoF) mechatronic testing systems. The most recent families of these systems involves various evolutionary incarnations of the 3-DoF NRL "In-Plane Loader System" (NRL-IPLS) and the 6-DoF NRL66.x systems. The most recent versions of these mechatronic systems as shown in Fig. 1.

In addition to these systems, high performance full-field displacement and strain measurement technologies were also developed to alleviate the inadequate sensitivity, accuracy and efficiency of other full field methods such as Digital Image Correlation. These technologies are the Meshless Random Grid (MRG) [10] and Direct Strain Imaging (DSI) [11, 12] methods [13]. These were integrated with the automated multiaxial testing frameworks and the appropriate inverse problem solution methodology to collect the necessary displacement and strain field data [14, 15, 16, 17, 3].

3. Characterization via the 3-DoF In-Plane Loader System

3.1. Specimen Considerations

PMCs associated with various applications range through a wide variety of constituent materials. Every distinct combination of matrix, fiber, fiber coating (for matrix-fiber interphase), layup angle, stacking sequence, etc. corresponds to a different material. Approximately 100 material systems with fibers ranging from Kevlar to IM7 graphite and several thermoset resins and thermoplastic organic polymers have been tested and characterized with the approach discussed here. A partial list of all the materials tested up to now can be found in [18]. The specimen geometry is described in detail [18, 19] elsewhere and was designed to satisfy the following requirements:

- The characteristic dimensions should be large enough relative to the fiber diameter and the lamina thickness to ensure that the material could be analyzed as either a single mechanically equivalent homogeneous anisotropic monolithic material, or a collection of layers of varying orientations of such materials.
- The overall specimen size should be small enough to keep material costs at a manageable level.

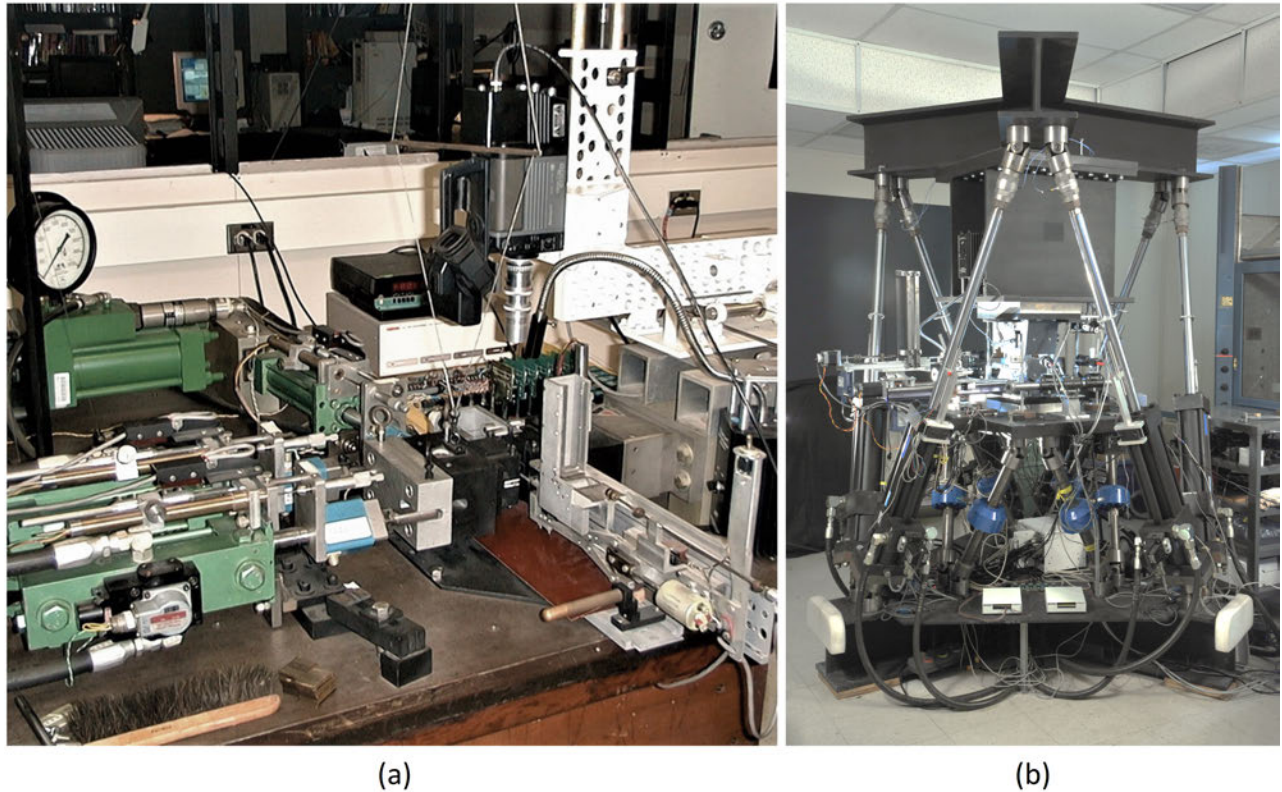


Figure 1. Long view images of the most recent versions of the 3-DoF NRL-IPLS (a) and 6-DoF NRL66.3 (b) multi-axial robotic testing systems.

- Strain riser(s) (such as notches, holes etc.) should be present to guarantee that high strain regions occur away from all gripping boundaries of the specimen.

3.2. Experimental Procedure

The main design objective of the IPLS is to control the rigid body motion of the one boundary of the specimen that is held by the movable grip while another grip holds the other boundary fixed. At the same time sensing subsystems measure the boundary displacements and tractions. Because the actuators of the IPLS are constrained to move in a plane parallel to the specimen, the resulting motion involves only three degrees of freedom relative to any frame of reference on that plane. As it can be seen in Fig. 2 the grip motion can be resolved into three basic components: sliding (shearing) u_0 , elongation (opening/closing) u_1 , and in-plane rotation u_2 .

Specified combinations of actuator displacements, therefore, map into particular combinations of these three basic motions. In order to visualize the loading space it is advantageous to think in terms of a three dimensional displacement space with coordinates (u_0, u_1, u_2) . The issue then is how to select a representative family of paths that cover the space and how to sample along each path. It was decided to cover the boundary displacement space with a set of 15 uniformly distributed radial loading paths as indicated in Fig. 3. Note that because of geometry

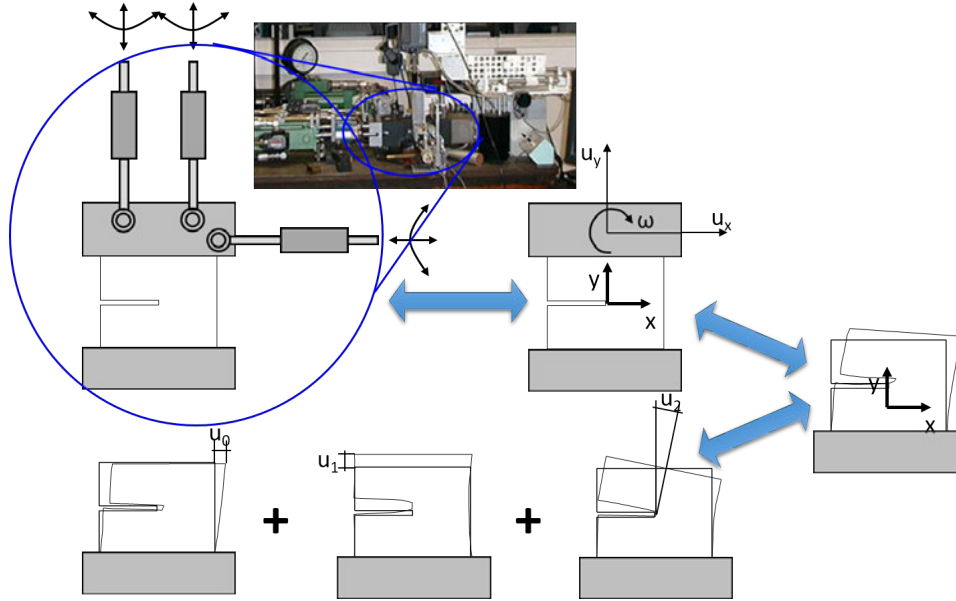


Figure 2. Loading Modes of the In Plane Loader Systems.

and material symmetry about the axis along the notch(es), only the half space corresponding to positive sliding displacement ($u_0 > 0$) need be considered. The required set of observation points is generated by sampling boundary displacement and force data along each path. A particular test in which the actuator motions are continuously varied corresponds to a specific path in this space. Assuming using one specimen per loading path implies that only 15 specimens are required, and 50 observations per loading path are obtained from a single specimen along the respective loading path. The locus of the end points of all loading paths for the same increment is a sphere as shown in Fig. 3(a), where three arbitrary loading paths are presented in a Cartesian frame spanned by with the polar coordinates in Fig. 3(b).

The process of computing the total dissipated energy (DE) due to strain induced damage is based on the boundary displacements and tractions that are measured at each increment imposed by the IPLS along each loading path. More details of the experimental procedure are presented elsewhere [18, 19, 20, 21]. One specimen per loading path is used initially and the procedure is then repeated for a total of two specimens per loading path.

3.3. Analytical and Computational Approach

The analytical approach followed is based on the conservation of energy and the additive decomposition of internal energy density of the material system under test. For a specimen of volume V in the absence of rigid body motion, for the case of quasistatic loads at the boundary that permit the elimination of inertial terms and in the absence of body forces, the conservation of energy can be reduced in the equivalence between the change of the internal energy being equivalent to the external work done as expressed by the form

$$\Delta U^{internal} = W^{external} \iff \int_{\partial V} w dV = \int_0^{u_i} t_i dq_i, \quad (1)$$

where U is the total internal strain energy and w is the internal strain energy density (energy per unit volume) and t_i, u_i are the tractions and associated displacements at the boundary, that are considered to be reduced to point forces for example measured by load cells. Allowing an

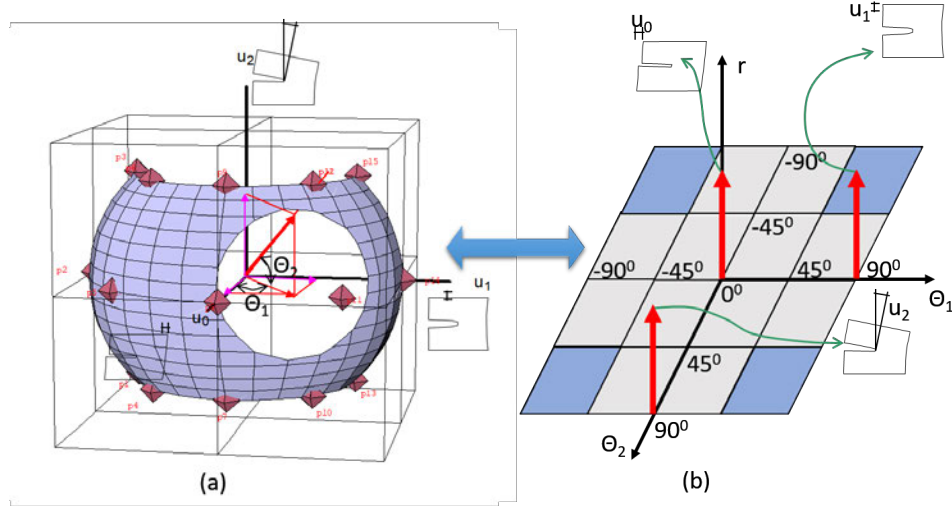


Figure 3. Loading Paths defined in the Cartesian space spanned by the basis modes (a) and corresponding unfolding of the truncated path surface in the spherical coordinates into a corresponding Cartesian system (b).

additive decomposition of the strain energy density to a recoverable w^R part that is assumed linearly elastic and an irrecoverable w^D (due to strain induced damage) or dissipated part ψ yields

$$w = w^R + w^D \iff w = \frac{1}{2} \sigma_{ij} \varepsilon_{ij} + \psi(\mathbf{d}; \varepsilon_{ij}), \quad (2)$$

where σ_{ij} and ε_{ij} represent the components of the Cauchy stress and infinitesimal strain second order tensors respectively and $\mathbf{d}$ represents a vector of material specific constants related to how the strains contribute to damage. Introducing Eq. 2 to Eq. 1 yields,

$$\int_{\partial V} \frac{1}{2} \sigma_{ij} \varepsilon_{ij} dV + \int_{\partial V} \psi(\mathbf{d}; \varepsilon_{ij}) dV = \int_0^{u_i} t_i dq_i. \quad (3)$$

Assuming that the equivalency between the internal energy and external work of the conservative part still holds (i.e. $\int_{\partial V} \frac{1}{2} \sigma_{ij} \varepsilon_{ij} dV = \frac{1}{2} t_k u_l$), the expression in Eq. 3 can be reduced to

$$\int_{\partial V} \psi(\mathbf{d}; \varepsilon_{ij}) dV = \int_0^{u_i} t_k dq_l - \frac{1}{2} t_k u_l = W^D, \quad (4)$$

where W^D represents the external work spent for dissipative processes due to damage evolution in the interior of the material and is measurable experimentally via force and displacement quantities that are measurable via the IPLS sensors. The expression in Eq. 4 enables the formation of an inverse problem for the determination of the material parameters in $\mathbf{d}$ that require the minimization of the objective function

$$J = \sum_{p=1}^{n_{Lam}} \sum_{l=1}^{n_{LP}} \left[W_{lp}^D - \left(\sum_{k=1}^m \psi(\mathbf{d}; \varepsilon_{ij}) \Delta V_k \right)_{lp} \right]^2, \quad (5)$$

where after a proper Finite Element Analysis (FEA) discretization of the domain in elements of volume ΔV_k with k indexing the elements, l indexing the n_{LP} loading paths and p indexing the

n_{Lam} distinct laminates made off the constitutive lamina under consideration. As mentioned earlier for the case of the IPLS based characterization, $n_{LP} = 2 \times 15 = 30$ and $n_{Lam} = 4$.

There are multiple ways to construct an analytical expression for the dissipated energy density (DED) function utilizing basis functions of the strain tensor components. The simplest is to consider it as a linear combination of strain components weighted by the n_B components d_r of the material parameter in $\mathbf{d}$ in the form

$$\psi(\mathbf{d}; \varepsilon_{ij}) = \sum_{r=1}^{n_B} d_r \chi_r(\varepsilon_{ij}). \quad (6)$$

Introduction of this expression in the objective function of Eq. 5 reduces the minimization problem to a typical L_2 norm optimization problem with the extra constrain that $\psi(\mathbf{d}; \varepsilon_{ij}) \geq 0$ imposed by the second law of thermodynamics. Computational implementation of this optimization enables the determination of all d_r that essentially determine the dissipative character of the material. Consequently, utilizing Eq. 6 the distribution of $\psi(\mathbf{d}; \varepsilon_{ij})$ can be plotted over the volume of the specimen. Typical distributions for two arbitrary loading paths and two basis load paths defined in the in plane load space is shown in Fig. 4. Two of them are

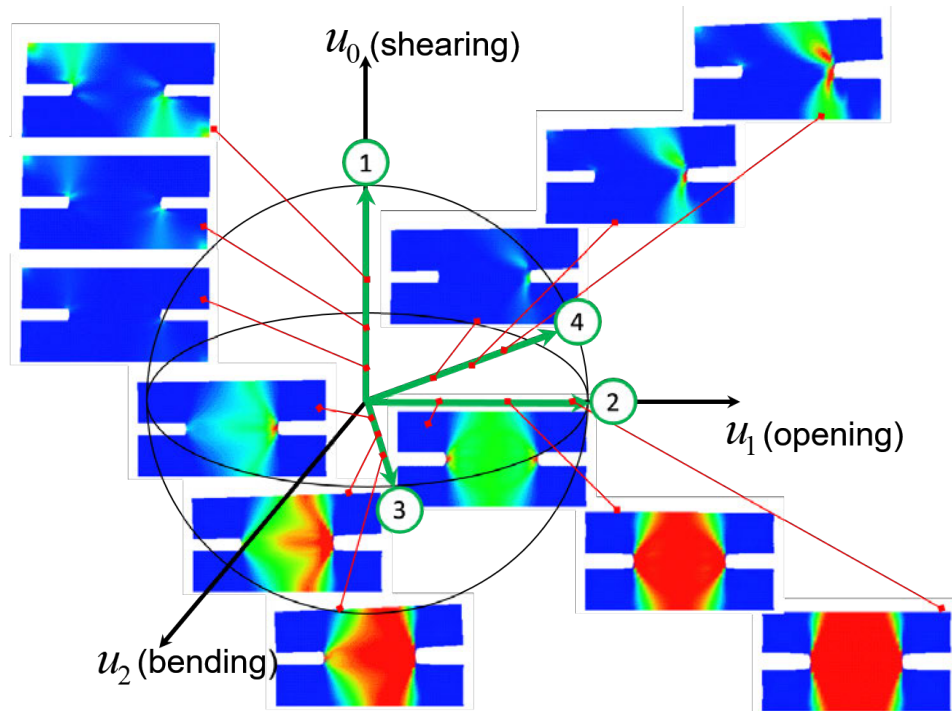


Figure 4. In plane loading space with post computed distributions of dissipated energy density of specimens at designated points of selected loading paths. Path ① involves only shearing mode, path ② involves only opening elongation, path ③ involves a linear combination of bending and elongation modes while path ④ involves all three modes.

the basis case for pure shearing (u_0) and pure opening elongation (u_1), one of them lies on the ($u_1 - u_2$) plane and one involves all three modes.

It is now trivial to compute the constitutive law as

$$\sigma_{ij} = \frac{\partial w^R}{\partial \varepsilon_{ij}} + \frac{\partial w^D}{\partial \varepsilon_{ij}} = C_{ijkl} \varepsilon_{kl} + \sum_{r=1}^{n_B} d_r \frac{\partial \chi_r(\varepsilon_{ij})}{\partial \varepsilon_{ij}}, \quad (7)$$

where C_{ijkl} represents the fourth order Hooke's tensor containing all the elastic constants of the material. Implementation of this law in a FEA code enables computing all quantities of interest involved in the structural mechanics problem associated with any composite that use laminae with the properties encapsulated by the material parameters C_{ijkl} and d_r . For a typical transversely isotropic material in a plane state of strain and for bilinear basis functions for ψ , the set of material parameters involves 4 elastic and 125 inelastic (i.e. dissipative) constants for a total of 129 material property constants.

4. Characterization via the 6-DoF NRL66.3 Loader

While the NRL-IPLS enables the dissipative characterization of composites dominated by in-plane states of strain and stress it does not provide any information about the out-of-plane behavior of thick composites exposed to simultaneous in-plane and out-of-plane states of strain induced by generalized 6-DoF loading conditions. Addressing this issue motivated the design of 6-DoF loader frames the most recent (third) version of them being the NRL66.3 as depicted in Fig 1(b).

The main differences in the analysis relative to that followed by the in plane approach exploiting the NRL-IPLS data, are the following:

- Instead of assuming that the elastic constants are known, the solution scheme was expanded to consider them as unknowns to be determined by the minimization of the objective function that in this case is formed in terms of the total strain energy density.
- To reduce the number of the unknown material parameters associated with the dissipative portion of the material behavior (i.e. the 125 coefficients mentioned earlier), we allowed certain material symmetries to hold beyond the elastic limit. This was achieved by employing a damage tensor that contains terms that correspond to those of Hooke's elastic tensor but that are weakening as a function of strain component magnitude.
- To enable the possibility of non-linear elastic behavior, in addition to the infinitesimal strain formalism, we also introduced a strain energy density hyperelastic formalism with damage involving large strains (Green strains) by integrating the two families of fibers model in [22] into the inverse characterization methodology.
- The space for defining the objective function required for the optimization for the parameter determination was expanded to include objective functions expressed in terms of strain tensor component distributions. This was enabled due to the fact that we developed high performance full field measurement technologies such as the MRG and DSI methods [13].
- The loading path space was chosen to be a 4-dimensional subspace of the full 6-dimensional (3 translations and 3 rotations) space that can be realized by the NRL66.3. This subspace is spanned by the 3 rotations and the opening-closing elongation. The hypersphere defined by the locus of the end points of the definable loading paths, is sampled homogeneously by 72 loading paths by proper programming of the NRL66.3.

These differences are in addition to the architectural differences between the NRL-IPLS and the NRL66.3. For more details on the constitutive characterization of PMCs by the use of the NRL66.3 system and associated solution of the relevant inverse problems, the reader is encouraged to explore [14, 15, 16, 17, 3].

The approach was validated against experimental data generated by testing of coupons that were used and data that were not used for the inversion process, and data from experiments

performed on composite specimens and parts of completely different geometries and stacking sequences than those of the characterization coupons [16, 17]. A typical example demonstrating the quantitative and qualitative accuracy of developed approach is shown in Fig. 5. The top row of images shows the strain tensor component field distributions from the front side of the specimen evaluated experimentally via the MRG method. The specimen has been loaded by the

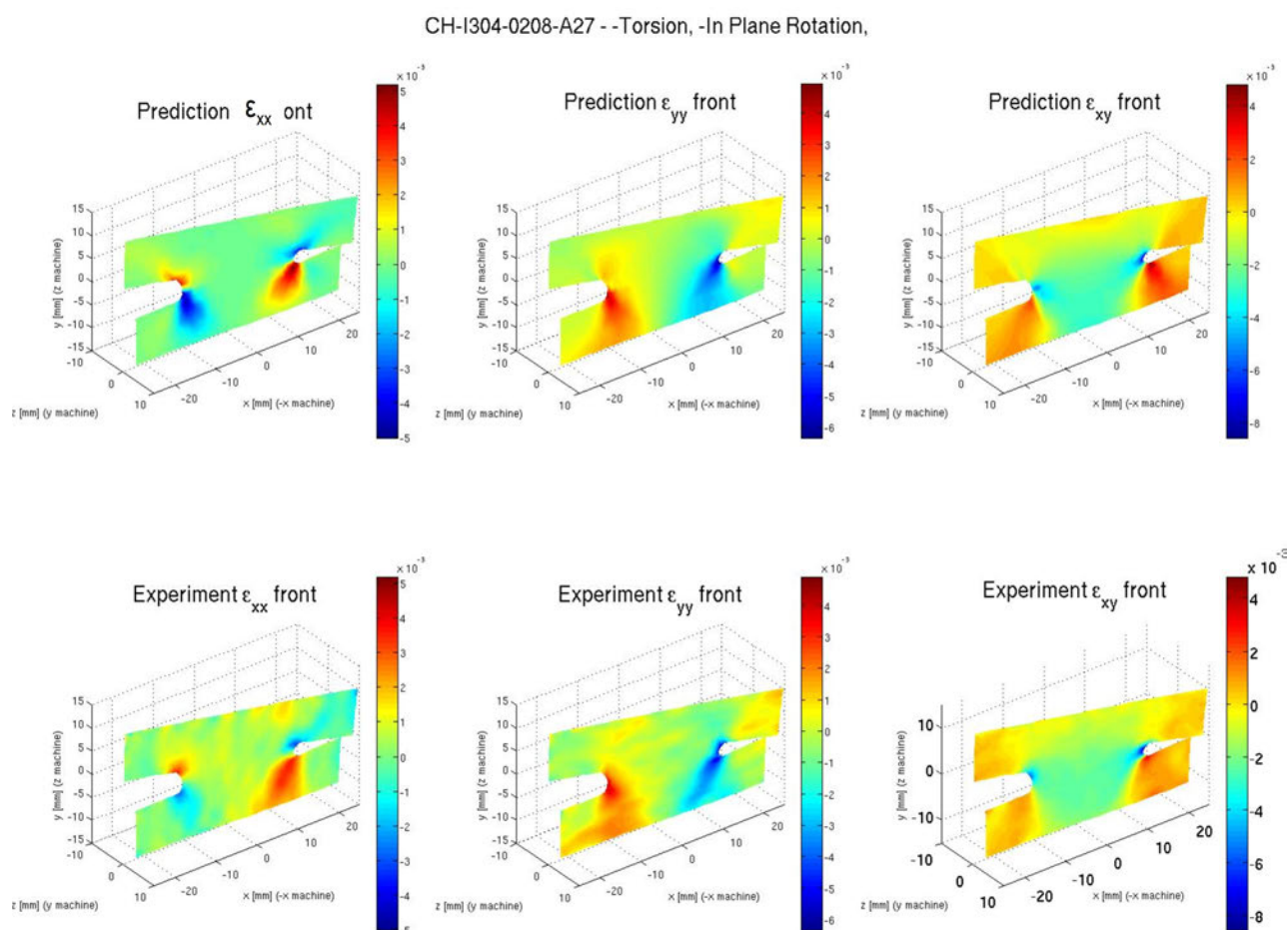


Figure 5. Top row: Distributions of strain tensor component fields measured experimentally on the front surface of a AS4/3501-6 $[\pm 30^\circ]$ PMC specimen coupon exposed to torsion and in-plane rotation by NRL66.3 and was not used for the material characterization optimization scheme. Bottom row: Homologous strain tensor component fields as predicted by the FEA that uses the identified constitutive model.

NRL66.3 under a combination of out of plane torsion and in-plane rotation. The displacements have been exaggerated by a scaling factor to reveal the deformation of the specimen that is a $[\pm 30^\circ]$ laminate of a AS4/3501-6 PMC system. The bottom row shows the corresponding distributions of the homologous strain component fields as predicted by FEA that uses the identified constitutive behavior. The detected deviation between experimental and predicted strain fields does not exceed 2% at any point of the domain and is on the order of the noise level of the experimental method.

5. Material Comparison based on Data-driven Dissipative Behavior

There are many processing parameters that can have significant effects on the structural properties of an advanced PMC, and on its suitability for various applications. Subtle variations between materials from different vendors can result in supposedly identical material systems exhibiting markedly different performance capabilities. Because of the limited ability to characterize and predict performance of composite materials under the combined loads experienced in structures, the US Navy has developed and follows an extensive series of characterization and certification tests as part of the development of a PMC material structure. This test series is valid only for the material system (and vendor) actually tested for a relevant application. Use of another vendor's material system requires repeating at least part of the qualification and certification testing. Because it is not clear which of these tests will show differences significant to the performance of the structure, often much of the test series must be repeated at great cost.

The US Navy has recognized the need to provide cost effective alternative sources for composite material systems. Alternative sources are essential to ensure competition in procurement and lower costs. It is also necessary to provide replacement materials in support of operational systems still in service, but made of materials no longer commercially available. The Office of Naval Research (ONR) specifically addressed this issue through the "New Materials, New Processes And Alternative Second Source Materials Data Base Generation And Qualification Protocol Development" program deployed in year 2000. This program was performed by a joint industry team lead by carbon fiber supplier BP-AMOCO. The team included prime airframe manufacturer Boeing, material suppliers Hexcel and Cytec-Fiberite, composite resin transfer molding part manufacturer GKN Westland, test laboratory Delsen, and data analysis company Materials Sciences Corporation in addition to US-NRL.

The BP team developed guidance in the form of a protocol defining the test matrix to characterize a new material for use on an existing structure. The guidance reflected judgment as to what constitutes a rational, cost effective set of tests sufficient to qualify the material for the application. The protocol considered the significance of differences between the substitution candidate and the qualified material. The greater the differences, the higher the apparent risk associated with the substitution and the more extensive the test matrix required by the protocol. A checklist of potential material application issues is provided, as well as guidance on test methods, number of replicates, and property values the replacement material must demonstrate for a successful qualification. The guidance considers not just mechanical properties, but also issues such as chemical compatibility and cost. In developing the protocol, the team performed selected material characterization tests to provide data and examples.

US-NRL was asked to apply its DE methodology to test materials manufactured in conjunction with the BP-AMOCO protocol development. The DE approach, through the automated multi-axial test machines, can rapidly generate a material characterization database. This was considered a good opportunity for US-NRL to demonstrate the convenience and utility of the methodology to the problem of second source materials.

5.1. Establishing Material Equivalence in Terms of Dissipative Behavior

The problem of determining whether two material systems are considered mechanically equivalent is different from (and much simpler than) the problem of deciding if a similar but perceptibly different material can safely be substituted in a specific structural application. Material equivalence has traditionally been approached by comparing characterization data. Identical characterization data has been taken to imply identical performance in any structural application. The term "identical" is used here in the sense of no statistically significant differences, given the repeatability of the material and test methods. If the characterization data is not identical, the new material may still be suitable for use in the structure. The

question then becomes how much further analysis and testing is required to demonstrate the material can safely be used in the structure and to re-certify the structure with the new material.

The traditional approach rests on an implicit assumption that the characterization methodology adequately captures all material responses critical to success or failure in the application. This assumption is rarely challenged; after all, we have been building successful composite structures for over five decades. However, a brief review of the evolution of materials characterization current practices, and the assumptions underlying them, does not necessarily support this assumption. The final report [23] of the previously outlined project has exposed insight as to why material characterization and second source certification have been proved such difficult and costly issues for composites.

Here we are focusing on material comparison aspects that are directly related to their dissipative behavior, in a way that does not rely on comparison of load-displacement curves along all the loading paths tested that would be analogous to the traditional approaches. We are rather focusing on a comparison based on an expressive data-reduction methodology that accounts for the multiaxiality mode interactions first at the entire structure level and then in the material level from the perspective of their dissipative behavior. This is achieved first by studying the distribution of DE at the structural level in terms of the loading mode combinations and secondly, at the material level in terms of the DED as a function of the strain state.

5.2. Dissipative Behavior Comparison at the Structural Level

For the purpose of identifying materials performance differences at the structural level a data reduction scheme is needed first. This data reduction and analysis approach is based on the multi-axial tests via the NRL-IPLS, we selected the data from testing specimens cut from Cytek's lot 372633, plate P2 made from T300 (RH) fiber and 977-3 resin laminae at a $[\pm 15^\circ]_8$ layup for the second source protocol project mentioned earlier.

As a first step the eight load paths that do not involve in-plane bending and therefore represent the cases of combinations of elongation (tension-compression) and in-plane shear that all lie on the 2D $(u_0 - u_1)$ plane are considered. Then the load displacement curves are constructed on the resultant planes $(\|f\| - \|u\|)$, where $(\|f\| = \sqrt{(f_0)^2 + (f_1)^2})$ and $(\|u\| = \sqrt{(u_0)^2 + (u_1)^2})$ are the norms of the component vectors for the forces and displacements respectively. Then we distribute these curves azimuthally on the $(u_0 - u_1)$ plane such as they all share the resultant force axis being normal to this plane. This operation defines a 3D space spanned by $(u_0, u_1, \|f\|)$ as shown in the upper left image of Fig. 6. The black lines represent the individual $(\|f\|, \|u\|)$ plotted on the azimuthally distributed planes corresponding to the respective paths defined on the $(u_0 - u_1)$ plane. An interpolation surface is constructed that passes from the $(\|f\|, \|u\|)$ distributions. This surface represents the continuous distribution of $\|f\|$ as a function of (u_0, u_1) . The upper right image in Fig. 6 shows the same surface color coded as a function of the force magnitude. Contours of equal force levels are also superimposed on this surface.

As a second step the tangential stiffness distribution surface is constructed by taking the derivative of the force interpolation surface with respect to $\|u\|$. This distribution along with the equal stiffness contours are depicted at the left bottom image of Fig. 6. Finally, as a third step the process is repeated to construct the surface of evolution of the DED W^D as a function of (u_0, u_1) and the associated contours as shown in the lower right image of Fig. 6.

A material comparison can now be performed by comparing the contours at a specific level of the corresponding quantities by using any of the three distributions depicted in Fig. 6. However, for the sake of brevity and to underline the difference in terms of the dissipative behavior we restrict the comparative analysis by using the DED distribution and specifically comparing the contours for a specific energy level corresponding to the materials of interest. Figure 7 shows the 0.1 lb.in contours of DE for two families of PMCs sharing the same 8552 resin but with different fibers (IM7 G and T650 G2). It is clear that not only there are very few areas that

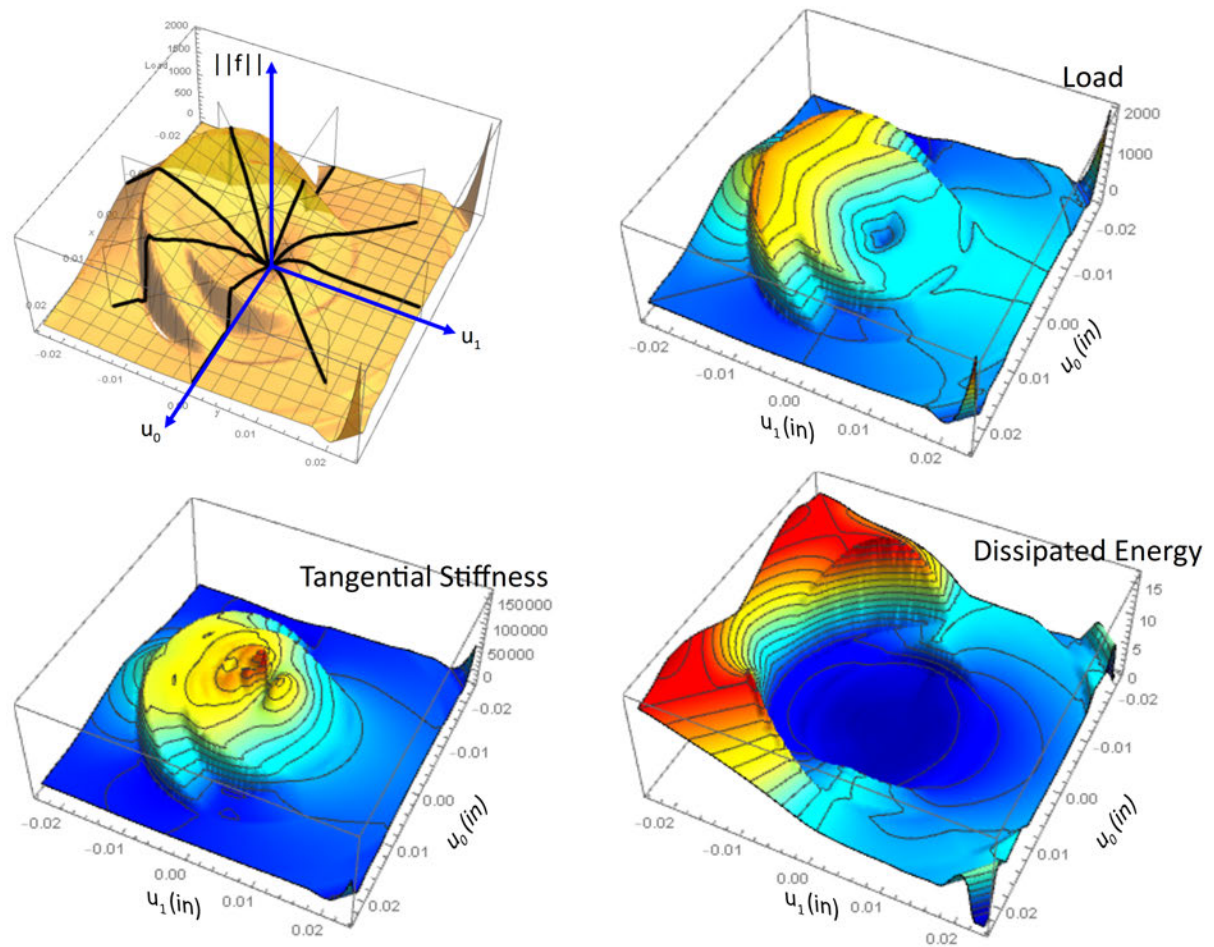


Figure 6. Top Left: Force resultants distributions along with corresponding interpolation surface. Top Right: Color coded and contoured load surface distribution. Bottom Left: Color coded and contoured tangential stiffness surface distribution. Bottom Left: Color coded and contoured dissipated energy density surface distribution.

the two PMCs are similar but the mixed mode behavior for the $[\pm 15^\circ]$ and $[\pm 30^\circ]$ layups is morphologically very different from each other, while the ones for the $[\pm 60^\circ]$ and $[\pm 75^\circ]$ layups present mostly scaling behavior for the mixed mode area. It is apparent that the difference of the elastic properties of the fibers are not sufficient for explaining the significant differences in these DE behaviors.

Figure 8 shows the 0.1 lb.in contours of DE for two families of PMCs sharing the same T650 G2 fiber but with different resins (3501-6, 8552, 977-3). This comparison indicates that the fiber properties can be associated with the close values in pure tension for most layups (for some cases for pure compression), but the resin differences have a much larger impact on the mixed mode cases, resulting to both morphological and scaling effects.

Figure 9 shows the 0.1 lb.in contours of DE for two families of PMCs sharing the same T300 fiber and the same 977-3 resin, but originating from three different production batches (Cy372633, Cy372636, Cy372637). Given that material is the same in all regards one would anticipate very small deviation of the respective DE contours. However, this is not the case and in particular, the most significant discrepancies appear in the region of pure closing compression)

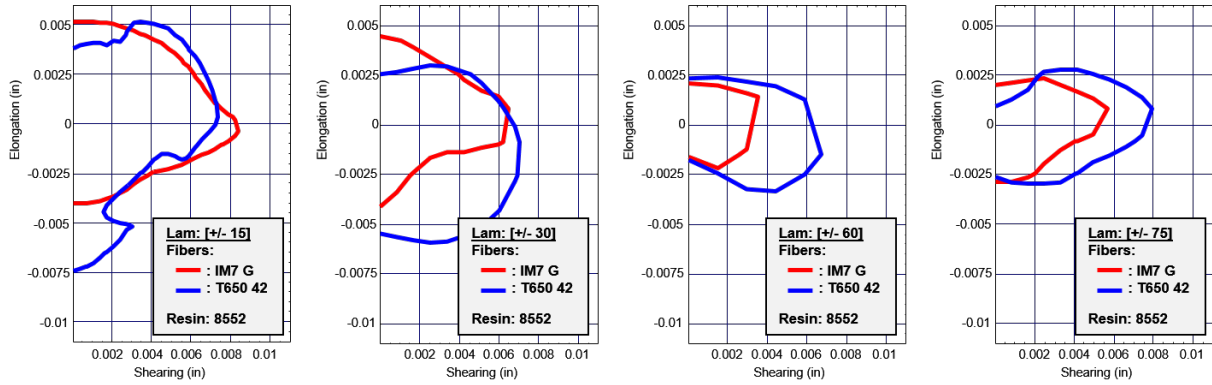


Figure 7. Contours of constant dissipated energy at 0.1 lb.in showing the effect of fiber variations within the same resin for four distinct layouts.

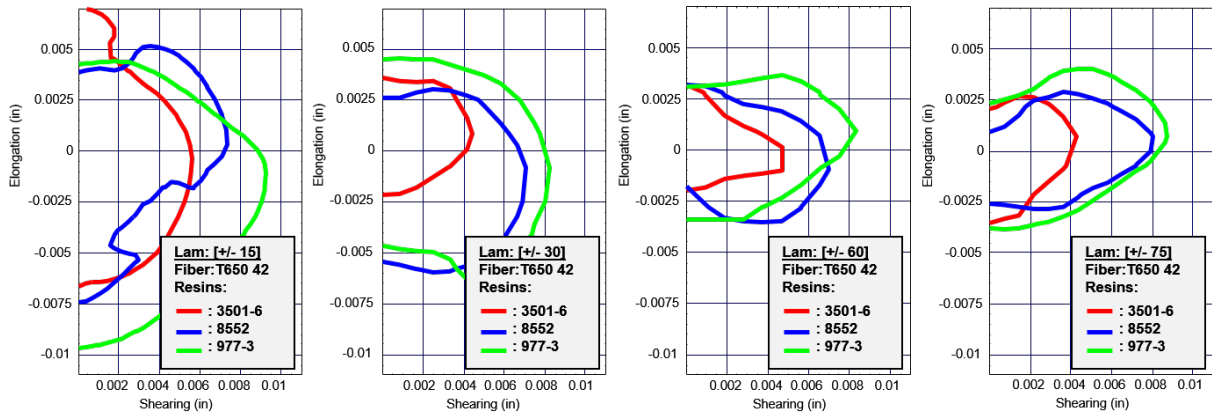


Figure 8. Contours of constant dissipated energy at 0.1 lb.in showing the effect of resin variations for the same fiber system for four distinct layouts.

and the regions of closing-shearing combinations for the $[\pm 15^\circ]$ and $[\pm 30^\circ]$ layouts.

These findings imply that if the level of DE is calibrated to correspond to the failure of the material in tension, batches Cy372633, Cy372636 could produce easily A- and B-basis allowables for the cases of $[\pm 15^\circ, 60^\circ, 75^\circ]$ since the contours at pure tension point coincide. However, that cannot be said for other areas where combined loading modes are present. This introduces the important consideration that even if one derives A- and B-basis allowables from uniaxial tests, it does not mean that the same specimens under biaxial load will also produce equivalent A- and B-basis allowables.

5.3. Dissipative Behavior Comparison at Material Level

For comparing materials without the effect of the structural geometry, it is necessary to turn attention on a quantity that describes the dissipative nature of the material in terms of quantities that do not depend on the shape of the structure but rather depend on the state of strain. Clearly, the DED function ψ satisfies this description. Since ψ is constructed to be a function of the local strains and captures the collective non-linear material behavior, it can be plotted in various strain planes to generate DED surfaces, in fashion similar to the one we followed for the DE in the structure. A typical example of the distribution of DED for three different laminates

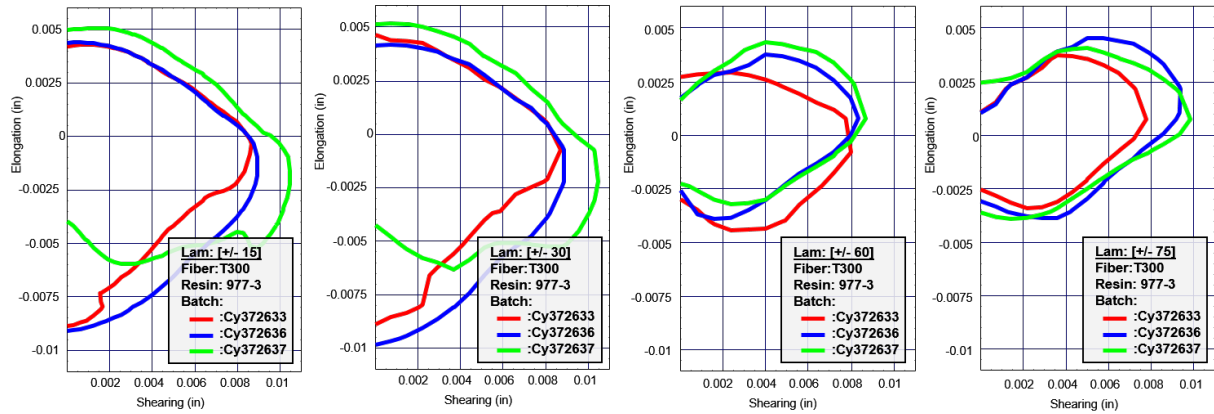


Figure 9. Contours of constant dissipated energy at 0.1 lb.in showing the effect of batch to batch variability for 3 different batches sharing the same resin and fiber systems for four distinct layups.

with plies from AS4/3501-6 system as shown in the top row of Fig. 10.

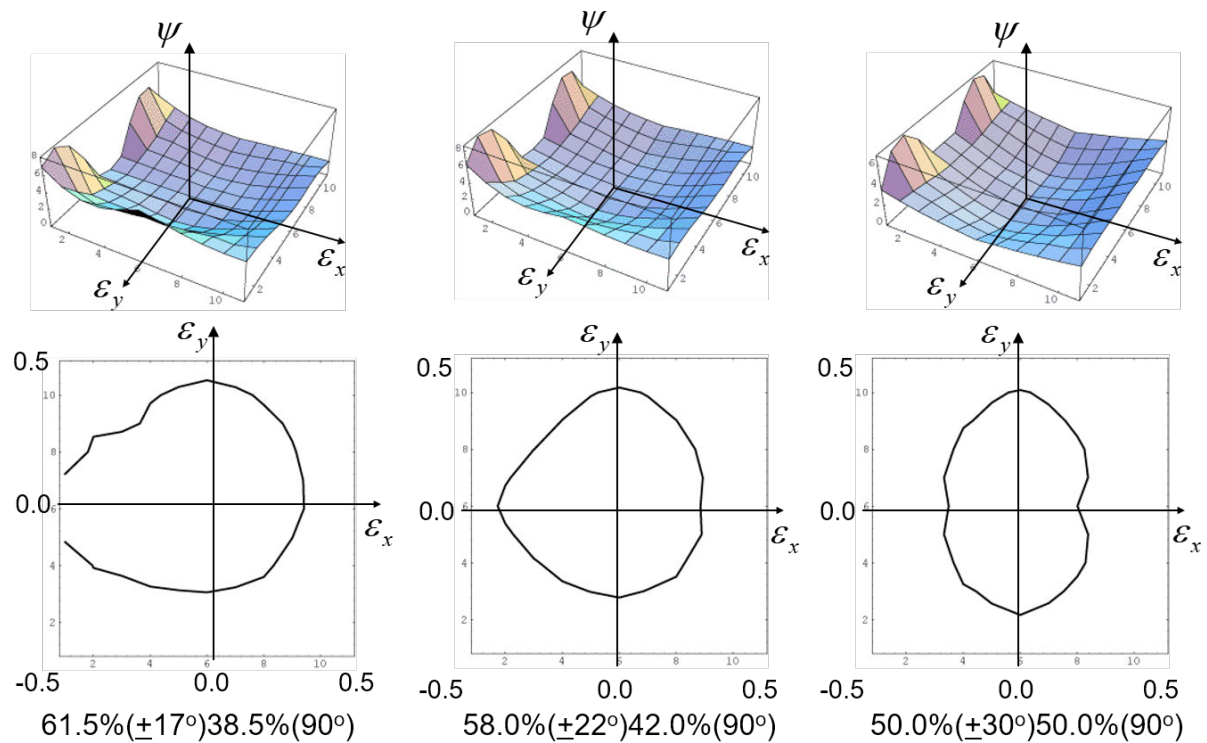


Figure 10. Dissipated energy density distribution as a function of the strains ϵ_x, ϵ_y for the case of $\epsilon_{xy} = 0$ (top row). Respective contours of constant dissipated energy density at 1 lb.in/in³ for the same layups.

Contours of constant DED can be extracted from the DED surfaces to obtain envelopes of criticality or failure (if one wishes to associate failure with a critical amount of DED) for each material system, as also shown in Fig. 10. Comparisons of these surfaces and/or contours

(or failure envelopes) can be used to determine the adequacy of the candidate materials to replace the qualified material in a particular application with respect to a particular metric for characterizing failure, namely a critical level of DED. It is evident that if the strain envelopes of the structure under consideration are available, then the suitability of the candidate material to safely satisfy the required strain performance can be easily determined without necessarily having to match the qualified materials performance.

If the suitability of the candidate material is still unclear, i.e. it is different from the qualified material but may be good enough to meet the design needs of the structure, then a detailed analysis of the structure of interest must be performed. At this point, the divergence between the two materials is such that the risk associated with the substitution becomes great. A database containing these types of DED representations would be applied to the structure through a structural simulation of the structure/material/load system. The structural performance of the system would be evaluated over all critical load conditions and the ability of the candidate material to satisfy the structural requirements determined. A successful simulation of the candidate materials ability to meet the requirement of the structure would greatly reduce the risk associated with the substitution. Further considerations would then need to be made to determine what appropriate structural verification testing would be required.

6. Towards Multiscale Inverse Problem

In an effort to assess how much information can be derived for material behavior at the micro-scale based on experimental data associated with the macro-scale tests, an inverse method for a cascaded model chain is presented. In order to achieve the inverse characterization of the composite material across multiple length scales, a representative volume element (RVE) of the composite structure at the micro scale was modeled, aiming to estimate the average properties of the heterogeneous media in the meso-scale (lamina). Consequently, the forward problem must first be formulated to enable the calculation of the homogenized properties of the given composite material. This material is assumed to have a structure consisting of parallel, cylindrical fibers, embedded in a polymer matrix and arranged in a periodic distribution, and packed in either a square or hexagonal array with a density reflecting realistic volume fraction of the fibers.

Subsequently, the properties estimated by the aforementioned homogenization process are considered as the properties of the lamina at the meso-scale, which in turn forms a balanced, angle-ply laminate at the macro scale. Synthetic experiments performed on the laminate include mechanical loading under 6-DoF conditions. These synthetic (simulated) experiments provide predictions of the associated strain fields. Solution of the inverse structural problem to estimate the micro-scale properties of the composite material may be accomplished using appropriate optimization algorithms, in order to enable the multiscale characterization of the composite material. This requires consideration of the homogenized response of the lamina at the mesoscale, as well as the laminate at the macroscale, utilizing experimental data collected at the macro scale.

6.1. Forward problem and mathematical homogenization

The three dimensional modeling of the composite microstructure outlined previously utilizes a micromechanics model that allows for the estimation of the full set of the elastic properties using a single model. This is in contrast to the conventional approach utilizing a collection of forward models, accompanied by scale-dependent assumptions, in order to estimate the full set of the properties needed. The problem of determining the material properties of heterogeneous materials such as composites, has long been studied [24, 25, 26] and many analytical homogenization techniques have been built based on the equivalent eigenstrain method [24]. These methods provide approximate estimates of the average elastic properties of the macroscopically isotropic and sometimes anisotropic heterogeneous material. However, in order

to comply with the transversely isotropic behavior that most composites exhibit due to the random distribution of fibers in the cross-section, an appropriate averaging procedure is used to provide a stiffness tensor with five independent constants corresponding to the transverse isotropy of the individual laminae.

The current implementation involves only numerical homogenization [27] through the use of finite element analysis, in order to work towards the inverse problem of composite characterization at the micro-scale of constituents (fiber and matrix) in a manner that follows the established methodologies as described in [28, 29]. The composite is assumed to be comprised of parallel cylindrical transversely isotropic fibers embedded in an polymer isotropic matrix. The microstructure is considered to be periodic and in either a square or a hexagonal arrangement, as shown in Fig. 11. In order to estimate the effective elastic properties at the meso-scale, the

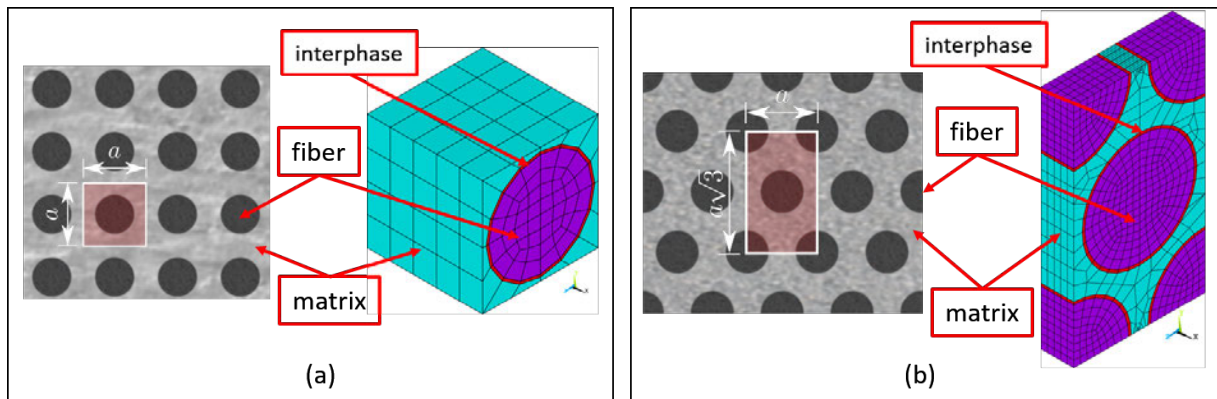


Figure 11. Mesoscale representation of composite lamina with tetragonal (a) and hexagonal (b) periodic fiber distributions along with equivalent FEA discretizations of respective RVEs required for homogenization.

composite is represented at the micro-scale by a 3D representative volume element (RVE), that is consistent with the arrangement of the constituents and is subjected to periodic boundary conditions [27].

Each RVE is subjected to an average strain $\bar{\epsilon}$ [30] and each of the six components of strain are applied by enforcing appropriate displacement boundary conditions through constraint equations at the faces, edges and the vertices of the RVE [28]. The volume average of the strain ($\bar{\epsilon}_{ij}$) is equal to the applied strain (ϵ_{ij}^{app}):

$$\bar{\epsilon}_{ij} = \frac{1}{V} \int_V \epsilon_{ij} dV = \epsilon_{ij}^{app}. \quad (8)$$

For the homogeneous composite, the average stress is calculated (in Voigt notation) by:

$$\bar{\sigma}_\alpha = C_{\alpha\beta} \bar{\epsilon}_\beta. \quad (9)$$

Consequently, the components of the Hooke tensor $C_{\alpha\beta}$ of the homogenized material can be determined by:

$$C_{\alpha\beta} = \bar{\sigma}_\alpha = \frac{1}{V} \int_V \sigma_\alpha(x, y, z) dV, \text{ with } \epsilon_\beta^{app} = 1, \quad (10)$$

where x, y, z are the spatial coordinates. A detailed description of the process alongside the necessary constraint equations that satisfy periodicity for each loading case can be found in [28]. The components of C_{ij} for the case of transverse isotropy are given by [31, 27, 32].

6.2. Multiscale Inverse Problem

As indicated earlier, in the single scale characterization framework [16, 33, 34] the inverse problem takes the form of an optimization problem. In that framework the forward evaluation is applied through a composed form of the models across various scales such that the usage of experimental measurements at the macro scale is naturally applicable. In the multiscale framework the constituents of the composite at the micro-scale are considered to be the matrix, the fiber and the interphase between the matrix and the fiber. The material properties for the matrix and the interphase have been assumed to be isotropic and transversely isotropic for the fiber. The properties in consideration are then defined as: E_m , ν_m are the Young's modulus and Poisson's ratio of the matrix, E_i , ν_i are the Young's modulus and Poisson's ratio of the interphase and E_{xf} , E_{yf} , G_{xyf} , ν_{xyf} , ν_{yzf} are the five independent engineering properties of the fiber. The set of properties is denoted as:

$$P = \{E_m, \nu_m, E_i, \nu_i, E_{xf}, E_{yf}, G_{xyf}, \nu_{xyf}, \nu_{yzf}\} \quad (11)$$

Since the aim of this work was to investigate the feasibility of identifying any subset of P : $U \subset P$ using an appropriate inversion scheme we can now define the set difference $K = P \setminus U$ as the set of known properties prior to characterization. When needed, the values of the properties in the set U can be identified by simpler experiments, for example a tension experiment to identify the matrix E_m and ν_m , or the fiber axial Young's modulus E_{xyf} .

It is anticipated that there will always exist elements of P that cannot be known a-priori. In the specific case of an RVE with an interphase layer between the fiber and the matrix these are the properties of the interphase (E_i , ν_i) that manifest only after the composite layers have been manufactured. In addition, sometimes determination of simple elastic material constants like the ν_{yzf} cannot be determined experimentally with high confidence.

In the form described herein, and with the aid of the definition of the forward problem, a block diagram of the multiscale inverse characterization process is presented in Fig. 12. The entire process is inside an optimization loop that takes the homogenized parameters and performs yet another forward evaluation of the meso- and macro-scale models. This process is performed for each load case that full field experimental data exist for. The strain results of the multi-scale forward analysis are then incorporated in an additive operation of objective functions. These objective functions are selected to be of the form,

$$f_k = \frac{1}{3N} \sum_{l=1}^N \sum_{i=x,y} \sum_{j=i,y} \left| \left[\varepsilon_{ij}^{exp_k} \right]_l - \left[\varepsilon_{ij}^{fea_k} \right]_l \right|, \quad (12)$$

where $|\cdot|$ denotes the absolute value, $\varepsilon_{ij}^{exp_k}$ are the surface strains measured at predetermined locations via a full-field measurement method [35, 36, 37, 38, 39, 40, 41, 42, 12] for the load case k , and $\varepsilon_{ij}^{fea_k}$ are the surface strains calculated from the forward finite element analysis of the load case k . l is the id number of the location the strain measurement takes place and N is the total number of strain measurement locations. An aggregate objective function $f = 1/K \sum_{k=1}^K f_k$ is used to collect the values of each of the objective functions evaluated for the specific load cases. It is important to note here that this approach still holds for the case of damage induced dissipative behavior of the structure that leads to reduction of the elastic properties.

6.3. Computational framework and synthetic experiments

The inverse methodology described in the previous section was implemented using MATLAB^{®2} as the control language and ANSYS[®]Mechanical^{TM 3} as the forward multi-scale evaluator.

² MATLAB[®] is a registered trademark of The MathWorks, Inc.

³ ANSYS, is a registered trademark of ANSYS, Inc.

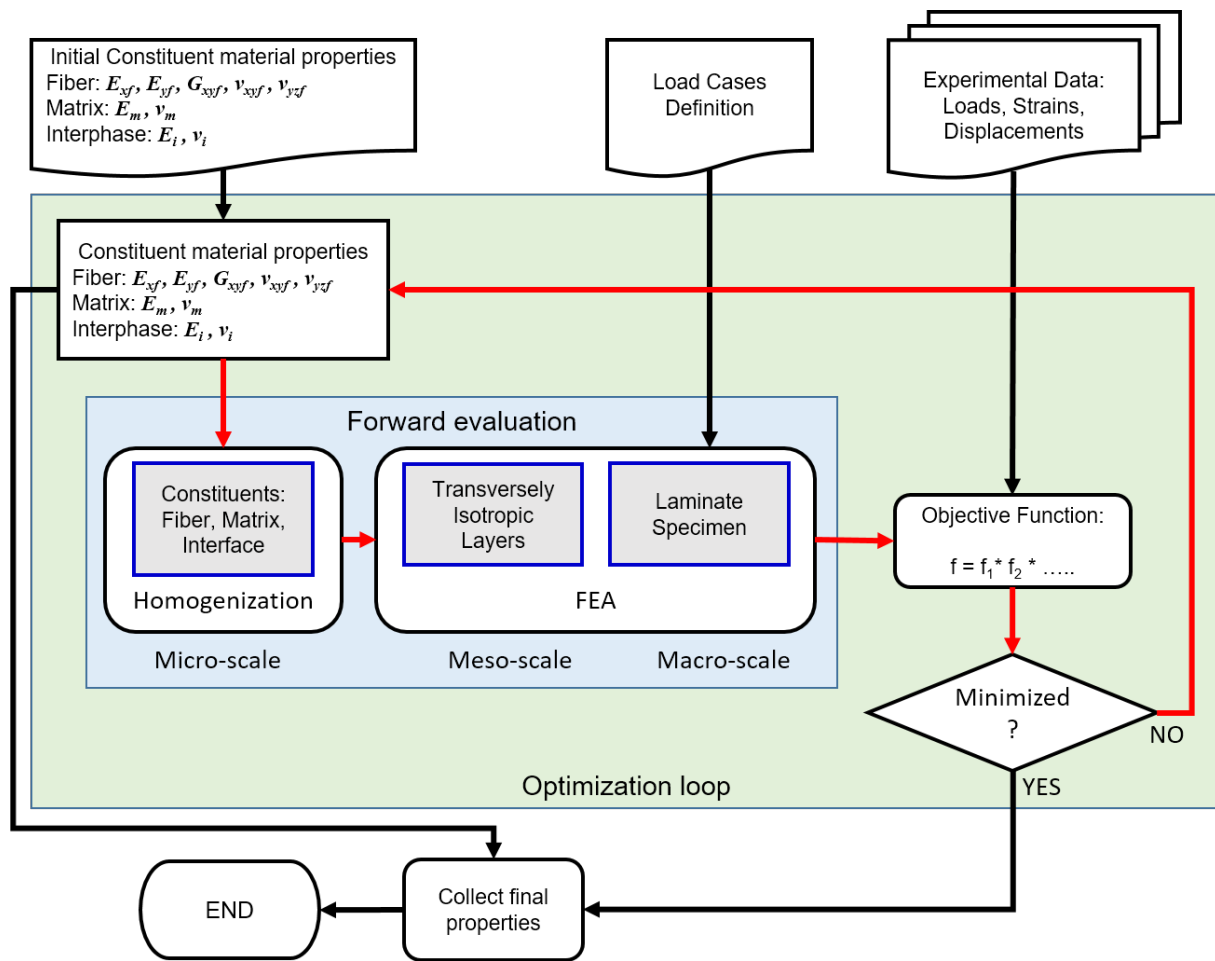


Figure 12. Block diagram of the multiscale inverse characterization process.

The connection between the two was achieved through an appropriate serial approach using file-system based exchange of information. Many optimization algorithms were explored as described in [32]. A non-linear derivative free global optimization algorithm with proper modifications to constrain the search space of the optimization parameters [32] was selected. Figure 11 shows the mesoscale geometry of both the square and the hex cells utilized with an interphase layer present between the resin and the fiber. The macro scale geometry is presented in Fig. 13(a). It has been discretized with hexahedral elements (SOLID185). A closeup at the area of the hole is depicted in 13(b) indicating that the composite material layers are modeled with a single element through their thickness.

6.4. Synthetic Experiments

In order to investigate the capabilities of the presented multiscale inverse method for characterizing a composite material at the constituents level by using data and the laminate level, we evaluated how accurately the elastic properties of the isotropic matrix and these of the transversely isotropic fiber can be estimated. This estimation was based on comparisons made relative to synthetic data that were generated by running the forward problem with known constituent properties.

All 128 possible combinations of properties appearing in Eqn. 11 were examined assuming

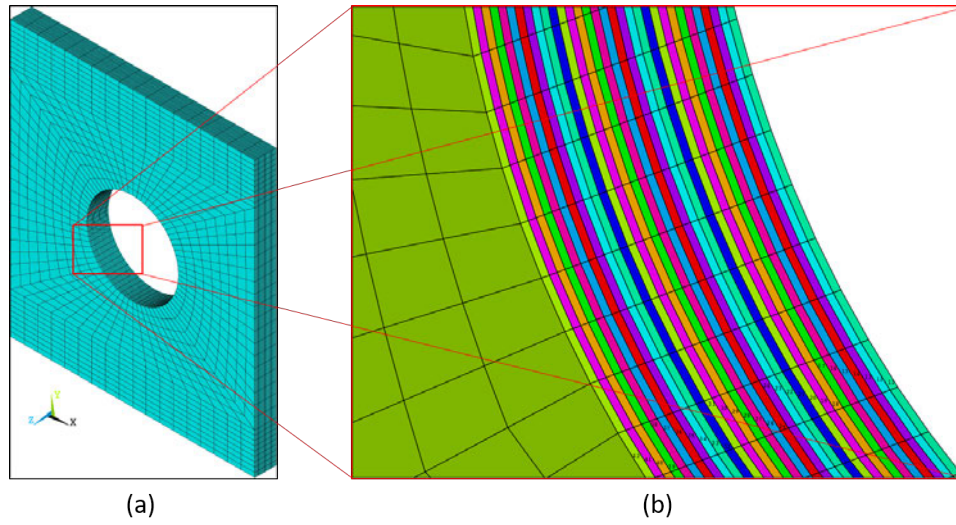


Figure 13. General view of the meshed macro-scale specimen (a) and close-up showing the meso-scale layer configuration of the meshed PMC specimen geometry with an open hole utilized for the synthetic experiments.

Table 1. Constituents material properties and optimization bounds

	E_m	ν_m	E_{xf}	E_{yf}	
Value	4.3GPa	0.35	235GPa	15GPa	
min	0.5GPa	0.0	10GPa	1GPa	
max	15.0GPa	0.45	600GPa	60GPa	
	ν_{xyf}	ν_{yzf}	G_{xyf}	E_i	ν_i
Value	0.2	0.07	27GPa	2.3GPa	0.25
min	0.0	0.0	1GPa	0.1GPa	0.0
max	0.45	0.45	75GPa	5GPa	0.45

that the interphase properties (E_i, ν_i) are always unknown. With regard to the macro-scale model, the laminate specimen dimensions were chosen to be: height 45 mm, width: 40 mm, thickness: 3.5 mm and hole diameter: 15 mm. For all the synthetic experiments, a single loading case was selected, defined in the full loading space of a 6 degrees of freedom loading vector acting upon the laminate at macro scale ([43]). The values of the components of this vector for the three force components and the three components of moment were: $F_x = 2241$ N, $F_y = 4310$ N, $F_z = 517$ N, $M_x = 3.45$ Nm, $M_y = 6.9$ Nm, $M_z = 69$ Nm. The magnitude of these loads was chosen to ensure that the developed corresponding levels of strain respect the linear elastic limits of the material model.

The composite material used to generate the synthetic results is the AS4/3501-6 carbon epoxy, with values of elastic properties of the fiber, the matrix and the lamina as they appear in [31] and also presented in Table 1, together with assumed properties for the interphase layer. The errors for each material property reported in the relevant tables were calculated using the formula:

$$e = \left| \frac{P_{inverse} - P_{nominal}}{P_{nominal}} \right| \times 100 [\%] \quad (13)$$

where $P_{inverse}$ is the value of the property identified by the multiscale inverse characterization

Table 2. Multiscale inverse characterization for selected cases of the square volume element with interphase layer synthetic experiments. Case IDs represent different choices of unknown parameters

ID	E_m	ν_m	E_{xf}	E_{yf}	ν_{xyf}	ν_{yzf}	G_{xyf}	E_i	ν_i	Evaluations	f (pStrain)
sia	-	-	-	-	-	-	-	< 0.1%	< 0.1%	124	2.3
sib	-	-	< 0.1%	-	-	< 0.1%	< 0.1%	< 0.1%	< 0.1%	1346	2.1
sic	-	0.13%	-	< 0.1%	< 0.1%	-	< 0.1%	< 0.1%	0.8%	3231	1.7
sid	0.3%	4.2%	-	-	-	1.2%	4.6%	0.65%	35.0%	2605	52.8

Table 3. Multiscale inverse characterization for selected cases of the hex volume element with interphase layer synthetic experiments

ID	E_m	ν_m	E_{xf}	E_{yf}	ν_{xyf}	ν_{yzf}	G_{xyf}	E_i	ν_i	Evaluations	f (pStrain)
hia	-	-	-	-	-	-	-	< 0.1%	< 0.1%	139	2.0
hib	-	-	< 1.3%	-	-	19%	10.4%	4.2%	52%	485	509910
hic	-	1.2%	-	< 0.1%	1.6%	-	0.6%	0.1%	6.3%	1430	2.1
hid	2.2%	7.1%	-	-	-	8.1%	4.6%	2.4%	35.4%	1485	347679

and $P_{nominal}$ is the value used to generate the synthetic data.

Starting by deploying the methodology described above and utilizing the associated computational framework for only one parameter and working our way up to the total number of unknown parameters and their possible combinations, we were able to obtain a maximum number of unknown parameters that can be concurrently defined with high accuracy. We have assumed an isotropic interphase zone, under the condition that the matrix and fiber properties are known. The parameter identification was successful, even for values of the interphase properties as low as 0.5 % of the matrix's elastic properties. In absence of noise in the synthetically generated data, the estimation of the interphase properties can be achieved with very low error.

In table 2 some interesting inversion results are presented for the case of the square RVE. In this table we observe that the interphase properties can be found with high accuracy if the properties of the other constituents are known, which may indeed reflect a realistic situation when constituent properties can be determined experimentally via separate testing. The same is true for other cases like the *sib* case. As the number of unknown increases the results are getting worse. The analysis of all 128 cases revealed that no case with over 6 unknowns was inverted efficiently.

The results of the hex RVE are presented in Table 3. It is observed that in this case the interphase properties are identified when they are the only unknowns. For other cases though the properties cannot be identified with satisfactory accuracy, besides the *hic* case. It should be noted that this is only a subset of interesting results and other cases have been solved with high accuracy. The value of this exercise lies on the fact that if strain induced damage causes certain reduction of the material properties at the micro-scale, then the approach proposed here has the potential to identify the values of the effective properties even for the case of these damaged materials.

7. Conclusions and Plans

The present work has outlined a data-driven methodology for executing multi-degree of freedom testing on composites, and subsequently identifying the constitutive behavior of such composites at the bulk lamina level by solving a properly formed inverse problem. As a natural extension of this process, the acquired data can enable the description of the dissipative behavior of

composites both at the coupon level (via dissipated energy) and at the material level (via dissipated energy density).

As an example of the utility of this view on the non-linear behavior of composites, it was demonstrated that material comparison has a considerably more complex phenomenology than can be expressed using only design allowables established by uniaxial experiments. Furthermore, it was shown that multiaxially loaded composites can exhibit drastically different behaviors in terms of dissipated energy despite appearing identical under uniaxial loading conditions.

In an effort to potentially identify damage effects at the micro-scale manifested as reduced mechanical properties in terms of experimental data acquired at the macro-scale, the present work also described a methodological framework along with its computational implementation. The feasibility of identifying mechanical properties of constituents of composite materials at the micro scale from experiments conducted at the macro scale was demonstrated by proper application of the proposed framework. The inversion methodology was applied to identify the properties of the interphase layer that develops between the matrix and the fibers of a PMC system. Both the Young's modulus and the Poisson's ratio were identified for the synthetic experiments conducted. Furthermore, it was also shown that it is possible to identify properties of other constituents as long as some of them are known via independently conducted characterization.

Plans for the future include a sensitivity analysis with respect to the constituent material properties, as well as the investigation of additional geometrical parameters as measures of damage evolution. It is also sought to incorporate the uncertainty of realistic (random) fiber distributions to eliminate the assumptions of periodic fiber arrays. The proposed methodology will be further enhanced by utilizing various global optimization methodologies in an attempt to establish a more detailed and efficient implementation of the inversion problem. The effect of adding additional loading paths in the optimization scheme (and the formation of the relevant objective function) will also be examined as potential means for both reducing the error of the characterized properties, as well as increasing the total number of the potentially identifiable properties. Finally, the methodology must be expanded to allow spatial variation of the degraded properties in a manner that frees the analysis from the implicit assumption that the identified properties are the same across the entire domain of the structure.

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