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Publication date:
2021-11-10

Permanent link:
https://doi.org/10.3929/ethz-b-000512194

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Originally published in:
Composites Science and Technology 216, https://doi.org/10.1016/j.compscitech.2021.108979

Funding acknowledgement:
150729 - Optical measurement of three-dimensional surface displacement fields of morphing structures (SNF)
Bending failure analysis and modeling of thin fiber reinforced shells

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ARTICLE INFO
Keywords:
Carbon fibers A.
Flexible composites A.
Computational mechanics C.
Failure criterion C.
Non-linear material

ABSTRACT
In this work, the impact of high stress gradients, found in bending of thin unidirectional fiber reinforced shells (~0.1 to 1 mm), on compressive micro-buckling failure, was analyzed. Such thin shells show increased resistance to compressive failure under high curvatures, which may even allow tensile fiber damage to drive ultimate failure for very low thickness (e.g. <0.5 mm). The main scope of this work is to analyze this increased resistance to compressive failure and propose a robust modeling scheme. The mechanical failure response was captured by a shell-buckling experimental campaign. The origins of the increased compressive failure resistance were initially attributed to the reduction of shear stresses acting on the most susceptible domain of a representative wavy fiber. This effect was effectively described by an analytically derived, stress-gradient-dependent parameter. The hypothesis for the establishment of this parameter was corroborated by a numerical micromechanical model adopting the embedded cell approach. This model also revealed important micromechanical interactions which were incorporated by simple stress and strain factors. The derived failure prediction scheme was further extended to include the non-negligible, non-linear elastic material behavior of carbon fibers by means of a numerical algorithm. The validity of the failure prediction model was demonstrated by the successful comparison with results acquired from the shell-buckling experiments on a unidirectional carbon-fiber reinforced epoxy system. To this end, the validity of the initial hypothesis of stress-gradient-dependence on compressive failure was corroborated. Major effect on the overall behavior modeling has carbon fiber’s material non-linearity, as well as micromechanical interactions.

1. Introduction & background in compressive failure of FRPs

Unidirectional (UD), fiber reinforced polymers (FRPs) are known to have lower longitudinal compressive than longitudinal tensile strength. Consequently, the bending strength is controlled by compressive failure. By contrast, thin shells (thinner than ~0.5 mm) subjected to bending, demonstrate remarkable resistance to compressive failure and experimental evidence shows that the tensile side fails first [1–3]. The origins of this unique behavior have not been identified for the time being. The subject of this work is the investigation of the sources of this particular behavior, using experimental evidence and mechanical modeling of the failure response.

The compressive failure behavior of UD FRPs of conventional thickness has been thoroughly analyzed with various experimental, analytical and numerical tools. The first widely accepted work that provided a predictive analytical scheme based on constituent properties, was done by Dow and Rosen [4]. In that work, buckling on fiber level, i.e. micro-buckling, was acknowledged as the reason for early failure of composites in compression. The adopted energetic approach provided closed form solutions to describe the two failure modes illustrated in Fig. 1a & b, namely, in-phase micro-buckling and out-of-phase micro-buckling. The former case is causing shear damage to the matrix (shear failure), while the latter causes a mixed damage mode (extensional mode) that is only expected for low fiber volume fractions, \(V_f\), of ~20–30% [4]. In well aligned FRPs, or composites of very brittle fiber/matrix interface (polymer or ceramic), transverse cracking due to Poisson’s effect may occur (see Fig. 1c), also leading to micro-buckling. Rarely, brittle fibers may fail in the maximum shear stress plane (Fig. 1d) at even lower strains.

According to Ref. [4], when neglecting terms of higher order, the compressive strength of a UD lamina due to shear failure mode, \(\sigma_{s,y}\), can be estimated by means of \(V_f\) and matrix’s shear modulus, \(G_m\), as: \(\sigma_{s,y} = G_m(1 - V_f)\). However, as indicated by Argon [5] and later thoroughly investigated by Kyriakides et al. [6], this approach stands as a very
optimistic upper bound (~4 times the experimental values [5]), since it is established for perfectly aligned fiber micro-structure. In reality, an existing initial misalignment causes important shear stress on the matrix even under pure compressive normal stresses. The shear failure of the matrix will initially lead to instability, and consequently to fiber bundle micro-buckling resulting in high bending curvatures of the fibers. The failure of the fibers forms the so-called, kink-bands [5,7]. Kink-band formation leads to significant reduction of the load bearing ability [6].

According to Argon [5], the shear stress on a misaligned composite bundle is \( \tau = \sigma_c \phi_0 \) (for small angles: \( \phi_0 \approx \sin \phi_0 \)), thus, a critical strength can be approximated as \( \sigma_{c,y} = \sigma_c \gamma_0 \), where \( \sigma_{c,y} \) is composite’s shear yield stress and \( \gamma_0 \) is a representative misalignment angle. About a decade after Argon, Budiansky [7] included the effect of local matrix transverse shear stress, \( \tau_T \), the local transverse & longitudinal normal stresses \( \sigma_T \) & \( \sigma_L \), and the created coupled stress due to moment, \( m \), as illustrated in the detail included in Fig. 1f. Such analysis can increase the accuracy on the predicted compressive strength, but leads to non-trivial differential equations that can be resolved using material constitutive laws. Moreover, existing analytical micromechanical schemes [7–11] contribute on the post peak-load response and the formation of kink-bands assuming an elasto-plastic matrix, while FE-based numerical schemes verify the sequence of failure events on the formation and damage progression of kink-bands [6,12].

All aforementioned schemes that consider some initial fiber misalignment, are able to approximate the experimentally acquired compressive strength values, which are usually close to the bending ones. A common compressive strain to failure due to micro-buckling is ~1 to 1.5% for FRPs [13], while the tensile ones are restricted by fiber’s maximum tensile strain limit. By contrast, thin shells (thinner than ~0.5 mm) subjected to bending, demonstrate remarkable resistance to micro-buckling and are able to sustain compressive strains as high as 2 to 3%, allowing the tensile side to fail first when fiber’s strain to failure is met [1–3].

The objective of the current study is to reveal the origin of the important resistance to compressive micro-buckling failure of thin shells under bending, compared to shells of conventional thickness, and propose a predictive scheme for their bending strength/failure curvature. The focus is applied on the compressive shear failure since transverse cracking (fiber splitting as in Fig. 1c) is shielded due to the limited development of Poisson’s effect at high curvatures [2]. Initially, a

Fig. 1. UD lamina longitudinal compression failure modes: a) In-phase micro-buckling / shear failure. b) Out-of-phase micro-buckling / extensional mode (\( \gamma_T \sim 20–30\% \)). c) Transverse matrix/interface failure due to Poisson’s effect. d) Shear fiber fracture. e) Detail of a): Shear stress and strain induced due to existing misalignment under homogenized compressive stress. Also schematized are the additional (actual and homogenized) shear strain & rotation \( \phi \) that \( \tau \) induces. f) Stress state around a representative ‘wavy’ fiber at the domain of the maximum waviness angle, \( \phi_{max} \), for remote uniform compressive strain field. Not to scale.
linear-elastic fiber response is considered to investigate the local stress interactions. Subsequently, this scheme is extended to incorporate the important non-linear behavior of fibers such as the carbon ones [2,14,15]. The predictions from the modeling scheme are compared with the results from conducted shell buckling experiments. The UD nature of the shells allows a clear isolation of the failure mechanism and material behavior. The overall analysis, the developed modeling scheme and corresponding results contribute to the robust design of foldable composites structures. The proposed failure modeling can be used for either purely UD FRPs or within first ply failure criteria. UD FRPs are expected to reach the maximum non-complex curvatures [16], nevertheless, they will not be able to sustain high complex curvatures due to the reduced transverse strength.

2. Experimental campaign

Thin shell flexure experiments, of UD carbon-epoxy thin coupons, were conducted using the shell-buckling test configuration [1,17]. The testing process followed is also meticulously described in Ref. [2], nevertheless, an outline of the essentials is included herein for completeness.

2.1. Material and specimens

Six different specimen series were produced from seven different plates with 4, 5, 10, 13-(two plates: a & b), 18- & 25- plies, made of 30 gsm thin ply Toray T700S carbon fiber prepreg, with TP402 epoxy resin (NTPT Switzerland), manufactured following the recommended autoclave cycle (initial dwell at 80 °C for 30 min and 2 h curing at 135 °C with 5 bar pressure) [18]. To assure full control of \( V_f \), the curing was done between two polished steel plates, while fine, hardened stainless-steel, precision gauge strips prevented over-compaction and controlled the thickness. A smooth surface finish, was provided by the use of 50 μm thick Polyimide release film (Airttech Thermallimide RCBS) [19]. Breather cloth or peel-ply were absent in this process as they would introduce considerable surface and thickness imperfections on the thin shell composites. The obtained laminates are of very high quality with practically no voids (very low porosity, below 0.5%), and very uniform through-thickness fiber distribution as shown in Fig. 2a. The resulted thicknesses were 130, 164, 335, 420 (13a), 589 and 800 μm with a mean standard deviations within each family of ±3–7 μm and a nominal cured ply thickness \( t_{ply} \approx 32.5 ± 0.5 \text{ μm} \), measured using digital optical microscopy (Keyence VHX6000). The corresponding \( V_f \), defined by the fiber mass content and the final thickness was 58.5 ± 0.5% for all, except for 13b-with mean thickness of 403 μm (\( t_{ply} \approx 31 \text{ μm} \) which was ~61%. The nominal \( V_f \) was verified using optical analysis (via Matlab®) and thermogravimetric analysis (Pyris TGA). The composite plates were cut into \( L \times B = 100 \text{ or, } 150 \times 40 \text{ mm}^2 \) specimens. The width, \( B \), was chosen as such to ensure uniform strain in that direction. The choice of length, \( L \), is related to plate tangency attainment (see Figs. 2b and 3c), buckling curvature at failure and image-acquisition-equipment’s depth of field that was used for the Digital Image Correlation (DIC). Consequently, the 18- and 25- ply specimens were longer. A fine airbrushed white paint layer was applied in all specimens on both sides, before applying a special stamp to randomly introduce black speckles (~170 μm²) that enable the DIC strain measurements.

2.2. Testing and strain acquisition

The thin shell-buckling configuration is illustrated in Fig. 2b. This shell buckling configuration allows for very high curvatures without complicated testing rigs, while the compressive forces are negligible compared to the dominant buckling induced bending [2]. Two aluminum plates were mounted in a Zwick Roell universal testing machine equipped with a 5 kN load-cell to measure the force, \( F \). The experiments were conducted at a constant displacement rate of 10 mm/min until coupons’ ultimate failure. In order to evaluate the strains and curvature on coupons’ surfaces, two dual camera setups (4 × ProSilica GT3400) were employed for the image acquisition (2 Hz framerate). A symmetrically inclined positioning enabled the essential 3D DIC scheme that can cope with the occurring large displacements. The acquired images were post processed using VIC-3D v7, to evaluate compressive and tensile strains on x-axis, \( \epsilon_{xx} \) & \( \epsilon_{xt} \) respectively, as well as the corresponding curvatures, \( \kappa_x \) & \( \kappa_t \), enabling the evaluation of the midline curvature, \( \kappa \) (see also [2]). All in all, the 3D DIC technique allows strain acquisition and curvatures of very high range in a remote manner (e.g. strain gages add thickness comparable to the specimens).

2.3. Characteristics of experimental response

Pictures of representative 10-ply and 18-ply specimens, acquired with the image acquisition setup, are shown in Fig. 3. Specimens up to 10-ply-thickness do show any discernible damage on the compressive side at the moment that pronounced failure occurs on the tensile side, evidenced by fiber tensile breakage, which later leads to distinct fiber split, attributed to fiber-matrix failure and pure matrix cracking. This can be seen with simple visual observation of the acquired pictures (Fig. 3) but also from the strain redistribution that can be evaluated during the DIC analysis (see also [2]).

On the contrary, the thicker specimen families such as 13 or 18-ply and above show a response similar to what is expected for specimens of conventional thickness (e.g. ~1–2 mm according to norms [20, 21]). In detail, in these thicker specimen families, compressive damage precedes and leads the failure. The damage comprises compressive fiber
4. Mechanical analysis and modeling

In order to identify the reasons why compressive micro-buckling/shear failure is suppressed in very thin shells, the mechanical analysis initially focused on the homogenized stress field around the $\phi_{\max}$ domain (Fig. 1f), acknowledging that thicker specimens followed the expected shear induced fiber microbuckling explained in §1. A linear-elastic approach allowed an analytical evaluation. FE-numerical micro-mechanics depicted the local stress field. Finally, the derived model was implemented in a numerical algorithm to incorporate the carbon fiber’s elastic, material non-linearity. The estimated stresses are compared with the strength of the matrix to predict failure.

3.1. Properties of constituents and homogenisation

During the analysis, the matrix (TP402 epoxy resin see §2) was considered isotropic with a modulus $E_m = 3.44$ GPa [18], while a shear modulus $G_m \approx 1.27$ GPa was evaluated for a typical Poisson’s ratio $\nu_m = 0.35$. At this stage of the analysis, a nominal tensile fiber modulus is considered (chord-modulus), $E_{11T} = 230$ GPa, and the nominal longitudinal tensile strain to failure is $\epsilon_{T-T} = 2.1\%$ [22]. Nominal fiber diameter $d_f$, is $7 \mu$m. The longitudinal composite’s modulus $E_{11}$, was evaluated using conventional rule of mixtures (ROM), when linear-elastic response was considered, i.e. $E_{11} = V_f E_{11f} + (1-V_f) E_m$. The remaining engineering constants were approximated using Halpin-Tsai micromechanical corrections [13] (\(\xi_2 = 2\) for $E_{22}$, \(\xi_2 = 1\) for $G_{12}$), with fiber properties by Ref. [23]. The corresponding calculated engineering constants for $V_f = 60\%$ are: $E_{22} = 8.2$ GPa, $G_{12} = 4.26$ GPa, $G_{23} = 2.68$ GPa, $\nu_{12} = 0.31$ & $\nu_{23} = 0.43$.

3.2. Meso-/micro-mechanics of shear failure micro-buckling under bending

In order to explore the load-state at the maximum shear region of a typical sinusoidal fiber misalignment, i.e. at $\phi_{\max}$, a ‘wavy’ fiber of diameter $d_f$ is considered, along with a matrix-rich zone of thickness $t_m$. Under pure compression, the domain around $\phi_{\max}$ is exposed to a compressive stress field $\sigma_c$ (homogenized), as in Fig. 1e and f. When the domain around $\phi_{\max}$ is exposed to pure bending conditions (see Fig. 4a), according to Euler-Bernoulli beam-theory for a linear elastic material, a
linear through-thickness stress distribution, \( \sigma(y) \), occurs, of a slope \( \alpha = t / (\sigma_{\text{m}} - \sigma_{\text{m}}) \), with \( \sigma_{\text{m}} = \sigma_{\text{m}} \) and \( \alpha = -1/(\kappa E_{11}) \), with \( \kappa \) denoting the implemented curvature. Here, \( t \) is the thickness & \( \sigma_{\text{m}}, \sigma_{\text{m}} \) are the maximum tensile and compressive stresses respectively.

When the bent section is thick enough, it can be considered that the compressive stress at \( \phi_{\text{max}} \) is practically \( \sigma_{\text{m}} \), explaining why the flexural strength is controlled by composite’s compressive failure in much thicker coupons (e.g. 1 or 2 mm as in norms [20,21]). Nonetheless, \( \phi_{\text{max}} \) appears at a distance \( y_0 = (d_f + t_m) / 2 + y_0 \), from the free surface (Fig. 4a & Eq. (2)). Thus, the compressive stress at \( \phi_{\text{max}} \) shall not be considered equal to \( \sigma_{\text{m}} \) when \( y_0 \) is comparable to the distance from the neutral axis, \( y_{\text{m}} = (t_f / 2) \) for linear elastic case. Typical values for \( y_0 \) vary from 1 to 10 \( \times d_f \), or ~7 to 70 \( \mu m \) for \( d_f \approx 7 \) to 70 \( \mu m \) [6,8,12], hence are important for thin shells of roughly \( t \leq 0.5 \) mm, while \( \lambda \) lies between 100 and 400 \( \times d_f \).

Considering the very first misaligned fiber from the surface in the 2D scheme illustrated in Fig. 4a, it is anticipated that the shear stress (that will cause shear yielding) around a fiber on the matrix-rich zone is proportional to the compressive stress, as in Ref. [5]. Thus, the shear stress gradient should be equal to the gradient of the compressive ones. Hence, the effective compressive bending stress that will cause shear yield at \( \phi_{\text{max}} \) for a linear stress distribution (y-axis) is: \( \sigma_\phi(0) = (\sigma_1 + \sigma_2) / 2 \) (Fig. 4a), while the Mean Value Theorem allows to estimate this effective stress as \( \sigma_\phi(0) = (1 / \gamma_0^2)(\sigma_0 - y_0) \), with \( \gamma_0^2 \) the stress gradient. This local compressive bending stress can be evaluated by the minimum stress due to bending (on the surface), reduced through the parameter: \( \xi = 1 - 2y_0 / t \) to incorporate the stress gradient. Therefore, the critical shear is defined as:

\[
\tau = \tau_{\text{max}} \phi_{\text{max}} (3)
\]

Hence, Eq. (1) can be reformulated to predict the bending strength of a UD composite as:

\[
\sigma_\phi = \frac{\tau_{\text{max}}}{(\phi_{\text{max}} + \phi)} \xi \equiv \frac{\tau_{\text{max}}}{(\phi_{\text{max}} + \phi)} \frac{\tau_{\text{max}}}{(\phi_{\text{max}} + \phi)}(4)
\]

with \( \xi = 1 - 2y_0 / t \) & \( y_0 = (d_f + t_m) / 2 + y_0 \).

The effect of thickness in Eq. (4) is illustrated in Fig. 4b. The insert in Fig. 4b provides a schematic representation of the stress gradient variation, due to thickness, at \( \phi_{\text{max}} \) region. To produce Fig. 4b, representative values of fiber waviness were assumed with \( y_0 = 15 \mu m \) & \( \lambda = 750 \mu m \) [9] resulting in \( \phi_{\text{max}} \approx 0.078 \) rad (4.45°). The interfiber, matrix-rich zone was evaluated for a typical hexagonal fiber packing by:

\[
t_m = d_f \left( \sqrt{\frac{\pi}{2 \sqrt{3} V_f}} - 1 \right)
\]

For \( V_f = 60\% \) and \( d_f = 7 \mu m \) (for T700S), \( t_m = 1.6 \mu m \), thus, \( y_0 = 19.3 \mu m \). Composite’s \( \tau_{\text{c}} \) was assumed equal to the ultimate shear strength of the matrix, \( \tau_{\text{m,max}} \). This approximation accounts for a fiber-matrix interface stronger than the pure matrix, under homogeneous shear. The strength \( \tau_{\text{m,max}} \) was estimated as 71 MPa, based on the experimental data in Ref. [24], for an epoxy system with very similar properties to TP402 (tensile strength 62 MPa & flexural strength 148 MPa, according to Ref. [18]). The adopted \( \tau_{\text{c}} \) value is in the range of measured shear strengths for such CF-epoxy systems [13]. It should be noted that the ultimate shear strength can be much higher due to fibers’ realignment when the ~45 tensile test value is considered [25]. Finally, \( \phi \) was considered equal to the shear strain \( \gamma_{\text{c}} \), which the composite will show at \( \tau_{\text{c}} = \tau_{\text{m,max}} \). At the ultimate shear stress (strength point), matrix’s secant shear modulus due to plastic deformation is \( \sim 0.5G_{\text{m}} \) [24]. The use of the latter leads to a homogenized secant shear modulus \( \beta G_{12} \), with \( \beta \approx 0.55 \). This approach renders \( \phi = \gamma_{\text{c}} = \tau_{\text{c}} / (\beta G_{12}) = 0.03 \). The evaluated \( \beta \)-ratio that depicts the modulus’ reduction due to yield, can be compared with the 0.7 proposed in Ref. [10].

As depicted in Fig. 4b, the bending strength due to shear failure on the compressive side by Eq. (4), tends to infinity as \( \xi \) tends to zero, i.e. for very small thicknesses where \( y_0 \) approaches the bending neutral axis. This increase of the resistance to compressive failure for low thickness allows the stresses on the tensile side to drive the failure when the critical strain (here 2.1%) is reached, as shown in Fig. 4b. Thus, a bifurcation point/critical thickness can be identified on the bending strength vs. thickness diagram, at which bending failure switches from tension-driven to compression/shear-driven. Such a behavior is captured in thin CF reinforced shells in Refs. [1–3] and herein for specimens up to 10-ply (~335 \( \mu m \)), where the failure is driven by fiber’s tensile strength. Use of Eq. (4) along with the condition for tensile failure provides a bending failure vs. thickness model for linear material approximation.

3.3. Numerical micromechanics

3.3.1. Embedded cell model description

In order to verify the validity of the assumptions considered to form
the stress gradient dependent parameter \( \xi \), a 3D numerical finite element (FE) model of the area of interest around \( \phi_{\text{max}} \), as illustrated in Fig. 5, was created in Abaqus Standard v6.14. This model adopts the embedded cell approach [26]. A cylindrical, wavy (\( \phi_0 = 15 \mu m, \lambda = 750 \mu m \)) fiber-bundle (7 fibers of \( d_f = 7 \mu m \)) of a perfect hexagonal packing (\( V_f = 60\% \)) was modeled explicitly and embedded in a homogenized composite section with a perfect interface. The modeled domain around \( \phi_{\text{max}} \) had a length (x-axis) equal to \( \lambda/5 \), a 75 \( \mu m \) height (y-axis) and a 250 \( \mu m \) width (z-axis), large enough to provide uniform strain.

For this model, linear elastic material and small deformations were considered to allow direct comparison with Eq. (3). The homogenized domain and the fibers were modeled as orthotropic materials with the properties mentioned in [3.1 and [23] respectively, while the matrix was isotropic with \( E_m, V_m \) (see [3.1]). The embedded cell/fiber-bundle is inclined by the \( \phi_{\text{max}} \) angle (i.e. z- & 3-axis) coincident in Fig. 5). Different linear strain distributions with a common minimum nominal strain on the surface, \( \epsilon_{\text{b,min}} = -2\% \) and slopes/curvatures \( \kappa = -2 \epsilon_{\text{b,min}}/t \), for \( t = 75, 100, 150, 200, 500, 1000 & 2000 \mu m \), were imposed on the modeled domain. These nominal strains were imposed via symmetric compressive displacements on the x-direction, \( u_x \), applied on faces A & B (face normals also in x-direction, see Fig. 5) providing homogenized engineering strains as \( \epsilon_0 = 2u_x/\lambda/5 \). This allowed for the implementation of an equivalent strain profile that conforms to the ones expected for this bending case. This framework allowed to evaluate the load-state of the \( \phi_{\text{max}} \) region for different thicknesses. For completeness the modeled domain was also imposed to pure compression conditions with \( \epsilon_{\text{b,min}} = \epsilon_x = -2\% \) (see Fig. 5), corresponding to \( t \rightarrow \infty \).

No further constraints were implemented on the remaining faces to allow the full development of the Poisson’s effect. The selection of \( \epsilon_{\text{b,min}} \) is indicative and cannot affect the validity of the results, since, small deformations (linear geometry) were assumed. The models were discretized in \( \sim 1,800,000 \) linear, reduced integration brick elements (Abaqus C3D8R) with the embedded cell having a finer mesh with \( \sim 1,800,000 \) linear, reduced integration brick elements. This shear stress profile in local coordinates (1-2-3 in Fig. 5), \( \tau_{12,m} \), within the matrix around fiber \( \Omega \) is shown in Fig. 7a as a function of central angle (Fig. 6b) and depicts a clear thickness effect. Remarkably, for very low thicknesses, the peak stresses around the fiber are significantly reduced, even for a \( d_f = d_f \) (see also Fig. 6a & b), while for thicker specimens this difference vanishes, demonstrating that the stress gradient effect becomes negligible after certain thickness.

Since typical polymer matrices are expected to have an elastoplastic behavior [24] under pure shear loading, it can be assumed that instability and fiber micro-buckling are triggered when most of the matrix on fibers’ circumference has entered the yielding regime. As seen in Ref. [27], \( \sim 80\% \) of the material around a fiber bears damage before instability. In this framework, the 2D approximation by means of Eq. (3), \( \tau_{12,c} = \phi_{\text{min}} \phi_{\text{max}} \xi (\gamma_0, \psi) \) (for homogenized shear stress field) is compared in Fig. 7b with the effective shear stress around fiber \( \Gamma \) from the embedded cell model, calculated as \( \tau_{12,m-effective} = 1/\Gamma \int_0^\Gamma \tau_{12,m}(\Gamma) d\Gamma \), where \( \Gamma = \pi d_f \), i.e. the circumference of the fiber. Fig. 7b shows that the parameter \( \xi \) can capture the thickness-effect tendency, but shows that \( \tau_{12,c} \) is way higher than the \( \tau_{12,m-effective} \). This shows that, even-though the local shear on the matrix is driven by the compressive stress, is also highly affected by the complementary stresses that contribute to the local equilibrium [10] (see also Fig. 1f). The latter is highly affected by the orthotropic nature of the fibers as depicted in Fig. 6d where \( \tau_{12} \) and \( \tau_{xy} \) are shown.

Detailed stress analysis on the domain around \( \Omega \), included in the SM document, showed that the maximum shear stress on this matrix zone, is about 30\% higher than the minimum principal (compressive) stresses and more than 5 \times higher than the maximum principal (tensile) ones. Thus, the maximum shear stress shall drive yielding, having accounted for the typical failure behavior of a polymer [24]. The distribution of the maximum matrix shear stress around \( \Omega \) \( \tau_{\text{max,m-effective}} \) is shown in Fig. 7a (bottom) and the effective one as a function of thickness, \( \tau_{\text{max,m-effective}} \), calculated via integration similar to \( \tau_{12,m-effective} \), in Fig. 7b. The latter follows the same trend as the 2D approach \( \tau_{12,c} \), but is lower by a (mainly) constant factor \( \chi_1 = \tau_{\text{max,m-effective}}/\tau_{12,c} \approx 0.58 \), also shown in Fig. 7b. For very low thickness, \( \chi_1 \) has lower values since \( \gamma_0 \rightarrow \gamma_{max} \) and the boundary of the embedded cell tends to the neutral axis.

For completeness, the simulation of the pure compression equivalent (\( t \rightarrow \infty \)) was re-launched accounting for geometrical non-linearity (NL) effects and its results showed that the non-linearity is well captured (~2% tolerance) by Budiansky’s hypothesis for the contribution of the additional misalignment due to loading [7], i.e. \( t/\tau_{\text{NL}} \approx \phi_{\text{max}}/\phi_{\text{max}} + \phi \). However, \( \phi \) from FE (see Fig. 6c as in Fig. 1c) is about 11 \times lower than the estimation by \( \tau_{12,c}/G_{12} \), suggesting a 2nd micromechanical factor, \( f_2 = 11 \). This difference originates from the fact that the misaligned fiber domain is not free to shear, but is

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**Fig. 5.** Embedded cell approach applied to investigate the effect of bending stress & strain gradient at the ‘\( \phi_{\text{max}} \)’ domain’ of a sinusoidal fiber misalignment; maximum homogenized applied strain: \( \epsilon_{\text{b,min}} = -2\% \). The strains were imposed via symmetric compressive displacements on the x-direction, applied on faces A & B.
constraint by the surrounding continuum composite. This interaction was also considered in Refs. [10, 11]. In summary, the results of the embedded cell model can be employed to revise Eq. (4) as follows:

\[
\sigma_{3y} = \frac{\tau_{12}}{r_1} \left( \frac{\phi_{\text{max}} + \phi'}{\xi} \right) \chi_1 \chi_2
\]

with \( \phi' = \frac{\tau_{12}}{r_1} \left( \frac{\phi_{\text{max}} + \phi'}{\xi} \right) \chi_1 \chi_2 \chi_1 = 0.58, \ \chi_2 = 11 \)

& \( \xi = 1 - \frac{2y_0}{t} \), with \( y_0 = \left( d_f + t_m \right) \)

Here, a first order approximation is done for the contribution of the additional misalignment due to loading and plastic deformation, \( \phi' \), which is assumed to be equal to the misalignment caused by plastic shear deformation of the matrix at the maximum stress, reduced by the constraints implemented by the surrounding material.

The factors \( \chi_1 \) (micromechanical stress) & \( \chi_2 \) (micromechanical strain) represent the investigated hexagonal packing with \( V_f = 60\% \) and are expected to describe the local stress state for material combinations with similar elastic properties (i.e. orthotropic fibers and polymer matrix). Sensitivity analysis of these factors over \( V_f \), fiber-packing pattern, matrix and fiber type may be the subject of future studies.

3.4. Compressive shear failure for non-linear material & experimental verification

3.4.1. Non-linear material model implementation

Important efforts have been applied in the past to provide a material...
modeling scheme able to represent the CF non-linear material behavior [1,3,14,15]. Recently, Schlothauer et al. [2] demonstrated that the formulation proposed by Northolt et al. [14], based on the load induced realignment of the graphite layers/planes, can be employed to depict the full extent (tension & compression) of the longitudinal elastic response of CF and consequently CF-composite. In detail, on fiber level, the longitudinal elastic strains \( \varepsilon_{1f} \), relate with the applied stress \( \sigma_{1f} \), following Eq. (7a) by Ref. [14]:

\[
\varepsilon_{1f} = \varepsilon_0 + g\left(\varepsilon_0 - \frac{\sigma_0}{E_0}\right) \left[1 - \exp\left(-\frac{\sigma_{1f}}{\sigma_0}\right)\right].
\]

(7a)

Here, \( E_0 \) is the initial longitudinal fiber modulus, \( \varepsilon_0 \) is the graphite layers’ in-plane modulus and \( g \) is the shear modulus between the graphitic layers. The inversion of Eq. (7a) can only take place by use of the Lambert function \( W(\chi) \) as:

\[
\sigma_{1f}(\chi) = \frac{E_0}{g} \cdot \frac{\epsilon_0 \cdot \chi}{1 - \exp\left(-\frac{\epsilon_0}{g}\right)}.
\]

(7b)

As described in Ref. [2], utilization of single fiber experimental data [28,29] allows for the evaluation of the constants in Eq. (7) for T700S fibers, rendering the following values: \( E_0 = 216 \, \text{GPa}, \varepsilon_0 = 228 \, \text{GPa} \) & \( g = 0.588 \, \text{GPa} \). Then, use of Eq. (7b) and ROM provides the longitudinal stress of a UD composite as \( \sigma_{1f} = \sigma_0 \cdot \Omega(\varepsilon_{1f}) + (1 - \Omega): E_0 : \varepsilon_{1f} \). The resulted longitudinal stress-strain response for a single fiber and the CF-composite are depicted in Fig. 8. Compressive strains up-to 5% are included in Fig. 8, since according to Refs. [28,29], CF elastic recovery is expected at least up to this strain level and at least up to \( \sim 2.6\% \) for the UD CF-composite as tested in Ref. [2]. Micro-buckling failure is not considered in Fig. 8. Note that any effects of compressive plastic yield on the matrix, that may appear at \( \sim 2\% \) strain [24], are masked in the homogenized curve while the dashed line corresponds to strains beyond 3% that have not been observed experimentally [2].

4. Verification of the model with experimental results

4.1. Fiber misalignment analysis

A fiber misalignment analysis was conducted following the technique described in Ref. [30]. The details and the parametric study that accompanied the analysis are included in the SM document. In brief, this analysis allowed the evaluation of the fiber angle distribution using material’s sections (see Fig. 10a) in fiber direction and an image processing algorithm. These sections were done after the test in the vicinity of failed areas, but far enough to ensure intact sections. The traced fiber angle \( \theta_i \), allows for the evaluation of the fiber misalignment measure as. The statistical analysis showed, as expected, that mean fiber angle is practically zero (\( \bar{\theta} \sim 0^\circ \)) while the mean standard deviation \( \sigma_\theta \sim 1.95^\circ \), which is in the range of findings of older studies (0.8° to 1.9° in Ref. [31]).

The summary of the most important results are included in Table 1. A mean misalignment angle from specimens of all tested thicknesses is \( \bar{\theta} \sim 1.42^\circ \). As explained in the SM document, the said fiber-waveform characteristics are representative ones that can be traced in microscopy on the tested composite system; nonetheless, a statistical analysis of waveforms is a very challenging task, also susceptible to the fiber tracing method (e.g. methods in Ref. [30] vs [31]).

4.2. Model vs. experimental results

The curvature at failure, \( \kappa_f \), per specimen family (identified as explained in the SM document) is shown in Fig. 11a. The plotted curvature values correspond to the curvature of the central region of the buckled shell, where the maximum curvature is expected, considering the expected buckled ellipsoidal shape. The corresponding tensile and compressive strains (by DIC) at failure are shown in Fig. 11b. Table 2 is summarizing the curvature at which failure occurs, the corresponding strains on the compressive and tensile surface, as well as the damage mechanism that triggers the failure. The thickness that compressive
failure starts to precede for this material and $V_f = 58.5\%$ is $\sim 420 \, \mu m$ (13a-ply), as seen in Table 2. Some specimens of this thickness showed almost concurrent tensile and compressive failure. For the 13b-ply specimen with higher compaction and $V_f = 61\%$, the compressive failure preceded in all specimens. In thinner specimens the tensile failure precedes, at strains around the tensile limit of the fibers, while in thicker ones the compressive microbuckling led to damage.

The corresponding curvature and strain response per thickness using the algorithm in §3.4, with $T700S/TP402$ properties (found in §3.1 & §3.2) and for a waviness of $y_0 = 15 \, \mu m$, $\lambda = 120 \times d_f$ that leads to a $\phi_{\text{max}} \simeq 4.1^\circ$, are also shown in Fig. 11. This value corresponds to the 95th percentile of angle misalignment according to the analysis. Although this angle appears high, it should correspond to a peak of misalignment expected to lie on the maximum inclination of a fiber waveform. The video of the 18-ply specimen in the SM, illustrates that isolated ‘fiber-blisters’ appear in the surface when the first load drop occurs, being followed by more fiber-microbuckling. Shortly after these events, ultimate failure follows, since the low thickness of the material cannot tolerate even a small amount of damage. The aforementioned sequence of compressive failure events is affected by the local variation of fiber waviness, which results in randomly formed blisters along the available surface. Therefore, the $\phi_{\text{max}}$ estimator that fits the experimental results, reflecting only a probability of 5% where fiber misalignment is of greater value than $4.1^\circ$, is a reasonable estimator assuming that a limited number of microbuckled fiber can shortly lead to ultimate failure.

Remarkably, the modeling scheme is successfully predicting the switch of the failure driving mechanism from tensile fiber rupture to compressive/shear yielding. This corresponds to the bifurcation points on the strain vs. thickness plot in Fig. 11b. In detail, before the bifurcation point, tensile fiber breakage controls failure and the maximum

---

**Table 1**

<table>
<thead>
<tr>
<th>Thickness</th>
<th>5-ply</th>
<th>10-ply</th>
<th>13-ply</th>
<th>18-ply</th>
<th>25-ply</th>
<th>Mean</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_i [^\circ]$</td>
<td>$1.9 \pm 0.2$</td>
<td>$2.05 \pm 0.2$</td>
<td>$2.0 \pm 0.15$</td>
<td>$2.05 \pm 0.05$</td>
<td>$1.85 \pm 0.05$</td>
<td>$1.95 \pm 0.1$</td>
</tr>
<tr>
<td>$\phi [^\circ]$</td>
<td>$1.33 \pm 0.2$</td>
<td>$1.50 \pm 0.2$</td>
<td>$1.44 \pm 0.1$</td>
<td>$1.49 \pm 0.1$</td>
<td>$1.31 \pm 0.3$</td>
<td>$1.42 \pm 0.2$</td>
</tr>
<tr>
<td>$\phi_{\text{max}}$ [°]</td>
<td>$3.95 \pm 0.4$</td>
<td>$4.15 \pm 0.45$</td>
<td>$4.15 \pm 0.3$</td>
<td>$4.35 \pm 0.05$</td>
<td>$3.85 \pm 0.2$</td>
<td>$4.1 \pm 0.3$</td>
</tr>
</tbody>
</table>

The confidence intervals refer to measurements taken from different positions along the strips cut from the specimens; refer to SM document for more details.
strains are thickness independent, while after this point the maximum strains decrease in a hyperbolic manner, which approaches an asymptote around 1 mm. Moreover, the modeling scheme is able to capture the effect of $V_f$ (assuming unchanged fiber waveforms characteristics) on the prediction of the failure tendency per thickness, as seen in Fig. 11a and b. The small difference in the maximum compressive strains at failure is attributed to the pure-bending approximation in the model instead of buckling induced bending (see also [2]). Yet, these small differences in Fig. 11b, are within the DIC results’ scatter & the confidence bounds of the non-linear material fit with Eq. (7a). The failure mechanism switch points are indicated in the $\kappa_y$ plot (Fig. 11a). There, no discernible curve bifurcation occurs.

The experimental evidence shows that failure will mainly occur at a region around the central domain of the specimens, where the bending curvature is the highest. As a result, on one hand, fiber tensile failure is expected to occur when a weak fiber (e.g. following a Weibull distribution) is subjected to its ultimate tensile strain. On the other hand, microbuckling failure occurs when a highly misaligned fiber/fiber band (herein Gaussian distribution) is exposed to critical compressive strains. For specimens where compressive damage (micro-buckling) leads to catastrophic failure, blisters become visually discernible the moment the load drop occurs. This is in agreement with the findings of [12] which show that instability of a critical/misaligned fiber-band, occurs soon after matrix shear yield initiates (matrix elasto-plastic response was modeled in Ref. [12]). Nonetheless, the yielding on the microscale of the critical/misaligned fiber-bands that leads to the first blisters, is not captured on the $P-\kappa$ plots (see Fig. 3 and SM document) and is only shown when micro-buckling and blister formation appear.

For completeness, the prediction with the linear material model and a nominal fiber modulus $E_{11f} = E_0$ is also shown in Fig. 11a. For small thicknesses with tensile failure, their differences are limited to ~15%. However, when compressive failure becomes the driving failure mechanism, the differences are much more pronounced. Moreover, the switch to compressive failure predicted with the linear model for $V_f = 60\%$ is at $t \simeq 100$ mm ($\kappa_y \simeq 0.10$ mm-1), while for the actual, non-linear elastic fiber behavior is at $t \simeq 285$ mm ($\kappa_y \simeq 0.17$ mm-1). The origin of this difference is depicted in Fig. 9b for $t = 285$ mm, where the compressive through-thickness stress-gradient and stress at $y_0$ can be seen.

5. Discussion and broader aspects

As thoroughly analyzed in §1, the choice of fiber waveform characteristics has a vast impact on the compressive/shear yield point prediction. To address this, the prediction algorithm was launched with different $\phi_{\text{max}}$ values that result from variation of $\lambda$ and a common $y_0 = 15$ mm. The results are shown in Fig. 12a. Remarkably, for $\phi_{\text{max}} \ll 3.9^\circ$, fiber tensile rupture is expected to drive failure almost up to $t = 0.8$ mm. In contrast, when a slightly higher waviness is considered i.e. $\phi_{\text{max}} \simeq 4.45^\circ$ (as in the embedded cell mode and in Ref. [9] as well as, in the range reported in Refs. [6,8]) compressive yield is expected to drive failure for $t \simeq 115$ mm. It is worth mentioning that for $\phi_{\text{max}} \simeq 4.45^\circ$ and $t = 1$ mm, the maximum compressive strain at failure is $\sim 2.0\%$, a value almost identical to the one reported in Ref. [32] for another PAN based CF (T800S)-epoxy system. In general a higher fiber ‘representative’ waviness shall be expected for the conventional fabrication processes with peel-ply or breather compared to the herein implemented process (§1, the choice of fiber waveform characteristics).

This aforementioned ‘representative’ waviness refers to the through-thickness waviness. The in-plane waviness is not expected to affect the bending behavior significantly, since the ‘wavy’ fibers/fiber bundles will be laterally constrained by their neighbors when the $V_f$ is high enough, as in out-of-phase micro-buckling in Fig. 1b. Contrary, through-thickness ‘wavy’ fibers/fibers and especially close to the surface, have no support from the free surface thus, tend to form the experimentally-observed ‘fiber-blister’ on the surface, once instability occurs (see also SM). This is in-line with the observations in Ref. [30].

The ‘representative’ waviness as $\phi_{\text{max}}$ should refer to a critical amount of ‘wavy’ fibers that lead to ‘fiber-blister’ formation on the
failure model described herein describes a significant strength reduction which is found for the investigated thickness-families and the adopted mental scatter. No particular thickness dependence of the misalignment surface. The spread of the ‘wavy’ fibers is responsible for the experimental scatter. No particular thickness dependence of the misalignment angle was found for the investigated thickness-families and the adopted fabrication process, as seen in Table 1. In general, fiber waviness originates from the intrinsic waviness of the prepreg/fabric and the one induced during the processing. Thus, some increase of the misalignment level with increasing thickness cannot be excluded, as mentioned in Ref. [31], for thickness steps of an order of magnitude higher than the ones experimented herein (e.g. from 0.8 to 8 mm). However, the failure model described herein describes a significant strength reduction up to −1 mm, but the predicted reduction is only ~5% from that thickness until 8 mm, assuming a constant $\phi_{\text{max}}$. A fiber misalignment angle increase with thickness, as mentioned in Ref. [31], can explain the bending strength reduction presented in Ref. [32] for thicknesses from 1 to 8 mm.

The fiber misalignment statistics which show, at least for the investigated thicknesses, that the fiber angle dispersion is more or less unchanged, allows for the use of one representative angle. The fact that the modeling scheme can capture the experimentally acquired failure with thickness dependence proves its robustness to capture the main trends.

These trends would have not been captured without the incorporated material nonlinearity. The non-linear elastic material behavior leads to reduction of the bending stiffness $E_{11} I$ with respect to the nominal one evaluated by $E_{11} I = E_0$. This effect is illustrated in Fig. 12b as a function of thickness and $\kappa_0$. This shows that the reduced bending stiffness of UD laminates (usually evaluated by the applied moment in standardized testing) compared to the tensile one, is due to: i) the compressive micro-buckling mechanism and ii) the compressive softening of CFs, such as PAN-based (see also [15]). The latter causes an up to 40% reduction for thicknesses where micro-buckling is absent (Fig. 12b). Indicatively, for 1 mm thick shells under pure moment, the presented failure prediction scheme would suggest an apparent bending strength of ~2 GPa (based on the total moment and assuming linear stress through thickness).

6. Concluding remarks

By revisiting the fiber micro-buckling formation modeling proposed by Argon [5] and refined by Budiansky [7], and by incorporating the high strain and eventually stress gradients seen in bending of thin fiber-composite shells, the resistance to compressive failure at high curvatures for low thicknesses, was explained. The key for the mechanical modeling was the consideration of the important stress reduction at $\phi_{\text{max}}$ domain with respect to the maximum one (on the surface) for low thicknesses that was described by the stress gradient parameter $\chi$. The initial hypothesis for the stress gradient effect was corroborated by computational micromechanical modeling. The FE based micromechanical model not only exemplified the validity of the adopted analytical scheme, but also provided micromechanical factors ($\lambda_1$ and $\lambda_2$) to incorporate the stress and strain variations at the matrix-rich domain around a fiber, versus the homogenized field. The effects of the microscale have a very high impact on the accurate prediction of the behavior, as also discussed in Ref. [10]. The material non-linearity of CFs necessitated a numerical algorithm to evaluate the exact stresses at the $\phi_{\text{max}}$ domain, since the closed form solution with parameter $\xi$ for linear material (Eq. (4)) is not any more valid. The proposed scheme was able to describe the experimentally observed failure behavior of thin UD CF-epoxy shells under high deformation flexion and could explain the switch in failure driving mechanism from compression to tension, found in very thin shells [1–5]. The proposed failure modeling can be used for either purely UD FRPs or within first ply failure criteria. This failure prediction scheme along with the non-linear elastic behavior modeling described in Ref. [2], can be employed to design durable, composite thin shells, subjected to high deformation bending. To do so, material’s elastic constants are needed (linear and non-linear) along with shear yield strength of the matrix. In the current study, the quasi-static matrix yield strength was considered to model the failure under quasi-static bending. Creep, environmental fatigue or other cyclic effects on the matrix, can be considered by adjusting matrix’s yield strength (see also [33]). Moreover, knowledge of the ‘representative’ fiber waviness is required. In summary, all aforementioned material parameters, ‘representative’ fiber waviness, material non-linearity, as well as micro-mechanical effects are required and need to be incorporated in a thorough modeling scheme to capture the behavior of the tested thin shells.

Further experimental campaigns can substantiate the applicability range of the proposed scheme and elucidate the sensitivity on the essential ‘representative’ waviness. Computational micromechanical studies can contribute in expanding the studied effects for different microstructures and fiber or matrix types. The shell buckling experiment used for the experimental campaign allowed for essential observations on the free surfaces and also the use of DIC. Other bending setups which allow very large displacements, such as the ones proposed in Ref. [3] or in Ref. [32], may allow direct moment measurements, nevertheless, particular care shall be devoted in the load transfer areas.

Author statement

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

This work was supported by the ‘SFA-Advanced Manufacturing’ grant of the ETH-board as well as the SNF REquip program, SNF206021 150729, for the acquisition of the DIC.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.compscitech.2021.108979.

References